Predictions of the Spectra of the Rare-Earth Ions Ce^{3+} through Yb^{3+} in the Two Sites of Ca$_5$(PO$_4$)$_3$F
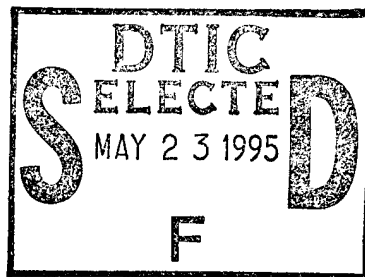
by Clyde A. Morrison

ARL-TR-708

DTIC
ELECTE
MAY 2 3 1995
F

April 1995

19950522 022

DTIC QUALITY INSPECTED 1

Approved for public release; distribution unlimited.

REPORT DOCUMENTATION PAGE

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE April 1995	3. REPORT TYPE AND DATES COVERED Interim, from 1 June 1993 to 1 Nov 1994

4. TITLE AND SUBTITLE Predictions of the Spectra of the Rare-Earth Ions Ce^{3+} through Yb^{3+} in the Two Sites of $Ca_5(PO_4)_3F$	5. FUNDING NUMBERS PE: 611102.H44
6. AUTHOR(S) Clyde A. Morrison	

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory Attn: AMSRL-PS-AA 2800 Powder Mill Road Adelphi, MD 20783-1197	8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-708
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory 2800 Powder Mill Road Adelphi, MD 20783-1197	10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES
AMS code: 21520406U6U01
ARL PR: 57E771

12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.	12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The results of fitting the experimental data on Er^{3+} in the two Ca^{2+} sites of $Ca_5(PO_4)_3F$ are used to predict the crystal-field parameters for the entire rare-earth series. These crystal-field parameters are then used along with the free-ion wavefunctions determined with aqueous parameters to determine a set of energy levels of the rare-earth ions Ce^{3+} through Yb^{3+} for both Ca^{2+} sites (Ca1 with C_3 symmetry and Ca2 with C_s symmetry) in $Ca_5(PO_4)_3F$. Also, the Judd-Ofelt parameters, Ω_k, are determined for each ion in the Ca1 and Ca2 sites, as well as the Zeeman g factors for the ground states.

14. SUBJECT TERMS Spectra, rare earths, calcium fluoroapatite (fluorapatite)	15. NUMBER OF PAGES 74
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT UL

1

Contents

Appendices

Tables

Tables (cont'd)

1. Introduction

Single crystals of $Ca_5(PO_4)_5F$ have been analyzed by x-ray diffraction, and the positions of all the ions in the unit cell have been determined [1,2]. The general space group information is given in table 1a. Since it is generally assumed that the rare-earth dopants replace the calcium ions, we see that of the 10 calcium ions in a unit cell, four are in the $4f$ position with C_3 symmetry and six are in the $6h$ position with C_s symmetry. The detailed x-ray data are given in table 1b. From the x-ray data in table 1b, the nearest neighbors to the Ca1, Ca2, and P sites were calculated; these are given in table 1c. These latter distances, particularly the Ca–Ca and Ca–P distances, are important in energy transfer considerations [3]. The crystal-field analysis assumes the crystal-field Hamiltonian of the form

$$ H = \sum_{nm} B_{nm}^* \sum_i C_{nm}\left(\hat{r}_i\right) , \tag{1} $$

where the B_{nm} are the crystal-field parameters, with $B_{nm}^* = (-1)^m B_{n-m}$ and $C_{nm} = \sqrt{4\pi / (2n + 1)}\, Y_{nm}(\theta_i, \phi_i)$. The $Y_{nm}(\theta_i, \phi_i)$ are ordinary spherical harmonics with polar angles θ_i and ϕ_i. In equation (1), the sum on n covers the even integers 2, 4, and 6, and the sums on i cover the number of $4f$ electrons, N, in the triply ionized rare-earth ion configuration $4f^N$. The sum on m in equation (1) depends on which Ca ion site the rare-earth ion occupies. For the Ca1 site with C_3 symmetry, the crystal-field parameters are B_{20}, B_{40}, B_{43}, B_{60}, B_{63}, and B_{66}. If B_{43} is chosen as real, then B_{63} and B_{66} are in general complex, and eight crystal-field parameters result. For C_s symmetry, the number of crystal-field parameters is the same as for C_2 symmetry; that is, B_{n0} for $n = 2, 4, 6$ and B_{22} are real, and the remaining B_{nm} are complex, making a total of 14 crystal-field parameters (Morrison and Leavitt [4], pp 86, 87). Having to deal with such a large number of crystal-field parameters, plus the complexities of two different sites, means that we must have very good starting values for B_{nm} in the analysis of the optical data. In both C_3 symmetry and C_s symmetry, I have adopted the convention that the lowest even-n B_{nm}, with m not zero, is real and positive; that is, for C_3, B_{43} is real and positive, and for C_s, B_{22} is real and positive (Morrison and Leavitt [4], pp 86, 87).

5

Table 1. Data on $Ca_5(PO_4)_3F$.

a. Crystallographic data: hexagonal C^2_{6h} ($P6_3/m$), 176, $Z = 2$.

Ion	Site	Symmetry	x	y	z	q
O1	6h	C_s	x	y	1/4	−1.8
O2	6h	C_s	x	y	1/4	−1.8
O3	12i	C_1	x	y	z	−1.8
P	6h	C_s	x	y	1/4	4.2
Ca1	4f	C_3	1/3	2/3	z	2
Ca2	6h	C_s	x	y	1/4	2
F	2a	C_{3i}	0	0	1/4	−1

b. X-ray data.

a (Å)	c (Å)	O1 x	O1 y	O2 x	O2 y	O3 x	O3 y	O3 z
9.3973	6.8782	0.4849	0.3273	0.4667	0.5875	0.2575	0.3421	0.0705
9.3684	6.8841	0.329	0.484	0.589	0.466	0.348	0.259	0.0730

P x	P y	Ca1 z	Ca2 x	Ca2 y	Reference
0.36895	0.3985	0.0010	−0.00712	0.24227	Hughes et al (1989) [2]
0.400	0.369	0.001	0.246	−0.007	Wyckoff (1968) [1]

c. Distance (Å) to any number of nearest neighbors, N, to Ca1 (C_3), Ca2 (C_s), and P (C_s) sites in $Ca_5(PO_4)_3F$.

Ca1 site Ion	N	R (Å)[a]	R (Å)[b]	Ca2 site Ion	N	R (Å)[a]	R (Å)[b]	P site Ion	N	R (Å)[a]	R (Å)[b]
O1	3	2.399	2.408	F	1	2.311	2.338	O3	2	1.532	1.511
O2	3	2.457	2.442	O3	2	2.348	2.376	O1	1	1.537	1.523
O3	3	2.807	2.753	O2	1	2.374	2.340	O2	1	1.538	1.534
P	3	3.207	3.190	O3	2	2.501	2.495	Ca2	1	3.075	3.067
Ca1	2[c]	3.44	3.45	O1	1	2.700	2.694	Ca1	2	3.207	3.190
Ca2	3	3.961	3.931	P	1	3.075	3.067				
				Ca1	2	3.961	3.931				
				Ca2	2	4.003	4.050				

[a]Hughes et al (1989) [2].
[b]Wyckoff (1968) [1].
[c]Average distance of two Ca1 ions.

2. Smoothed Crystal-Field Parameters for Ce^{3+} Through Yb^{3+}

The crystal-field parameters used in the first analysis are

$$B_{nm} = \rho_n A_{nm} \,, \tag{2}$$

where the radial factors ρ_n have been tabulated by Morrison and Leavitt [5], and the crystal-field components A_{nm} are calculated from the x-ray data [6]. For this analysis, I calculate only the monopole A_{nm} given by

$$A_{nm} = -e^2 \sum_j q_j \frac{C_{nm}\left(\hat{R}_j\right)}{R_j^{n+1}} \,, \tag{3}$$

where q_j is the effective charge (in units of electronic charge) on the ion at R_j. The x-ray data given in table 1b, along with the effective charges in table 1a, are used to compute the A_{nm} for the C_3 site (table 2) and for the C_s site (table 3). The A_{nm} in table 2 have been rotated about the z-axis (crystalline c-axis) so as to make A_{43} real and positive [4]. Similarly, the A_{nm} of table 3 have been rotated about the same axis so as to make A_{22} real and positive. The effective charges on the oxygen (–1.8) were chosen from the best fit to the experimental A_{nm} for triply ionized rare-earth ions in $Y_3Sc_2Al_3O_{12}$ [7]. The values of A_{nm} given in tables 2 and 3 with ρ_n for Er^{3+} were used in equation (1) to provide starting values for the C_3 and C_s spectra. The free-ion parameters were the same as used previously, and details of the fitting procedure are given elsewhere [8]. The irreducible representations for both C_s and C_3 symmetry are chosen from Koster et al [9]. The best fits to the experimental data for the C_3 site and the C_s site are given in tables 4 and 5. (These results have been previously reported but are included here for completeness [10].) Assuming that the A_{nm} are only host dependent, the best-fit B_{nm} can be used in equation (2) to produce experimental crystal-field components, A_{nm}^{exp}, by

$$A_{nm}^{exp} = B_{nm}\left(Er\right)/\rho_n\left(Er\right) \,, \tag{4}$$

and by using equation (2) again, we have

$$B_{nm}\left(X\right) = B_{nm}\left(Er\right)\left[\rho_n\left(X\right)/\rho_n\left(Er\right)\right] \,, \tag{5}$$

where X is any rare-earth ion. This calculation has been done, and the results are given in table 6 for the Ca1 site (C_3 symmetry) and in table 7 for the Ca2 site (C_s symmetry) and are referred to as the smoothed crystal-field parameters.

Table 2. Monopole (point charge) crystal-field components, A_{nm} (cm^{-1}/Å^n), for Ca1 site, C_3 symmetry, in $Ca_5(PO_4)_3F$.[a]

$n\ m$	ReA_{nm}[b]	ImA_{nm}[b]	ReA_{nm}[c]	ImA_{nm}[c]
1 0	9184	—	11980	—
2 0	7142	—	7310	—
3 0	190	—	82.2	—
3 3	2330	2444	2129	–2802
4 0	–3795	—	–3900	—
4 3	1617	0	1761	0
5 0	–566	—	–596	—
5 3	–593	2714	–622	–2637
6 0	–755	—	–740	—
6 3	575	84.7	560	–164
6 6	–107	–246	–73.9	224
7 0	81.0	—	63.3	—
7 3	–55.6	1.50	–46.4	–147
7 6	–63.6	215	–83.4	–202

[a]Rotated so that A_{43} is real and positive.
[b]Wyckoff (1968) [1].
[c]Hughes et al (1989) [2].

Table 3. Monopole (point charge) crystal-field components, A_{nm} (cm^{-1}/Å^n), for Ca2 site, C_s symmetry.[a]

$n\ m$	ReA_{nm}[b]	ImA_{nm}[b]	ReA_{nm}[c]	ImA_{nm}[c]
1 1	–5252	–1142	–2852	–3017
2 0	7900	—	9481	—
2 2	1442	0	2110	0
3 1	270.7	3119	2822	–1716
3 3	–1980	–3204	1746	–3041
4 0	1850	—	2031	—
4 2	–2920	–1644	–2314	2428
4 4	829	2104	–487	–2189
5 1	–50.90	1924	1703	–1066
5 3	1150	441.6	–1123	462.7
5 5	–855.2	139.7	–574.0	639.5
6 0	47.3	—	90.8	—
6 2	293	–257	389	197
6 4	170	–103	171	–10.4
6 6	–169	–136	57.1	161
7 1	–3.344	99.30	103	–81.96
7 3	–139.8	–212.8	117.7	–216.8
7 5	–28.10	46.53	–50.28	10.45
7 7	–202.1	82.33	–19.47	–207.6

[a]Rotated so that A_{22} is real and positive.
[b]Wyckoff (1968) [1].
[c]Hughes et al (1989) [2].

8

Table 4. Experimental and best fit theoretical energy levels of Er^{3+} in C_3 site in $Ca_5(PO_4)_3F$.[a]

$^{2S+1}L_J$ centroids (cm^{-1})[b]	Level	Γ_n	Energy (cm^{-1}) Theor.	Energy (cm^{-1}) Expt	Free-ion mixture (%)
$^4I_{15/2}$ (223)	1	$\Gamma_{4,5}$	−0.7	0.1	$99.91\,^4I_{15/2} + 0.04\,^4I_{13/2} + 0.01\,^4F_{9/2}$
	2	$^2\Gamma_6$	19.2	18	$99.90\,^4I_{15/2} + 0.06\,^4I_{13/2} + 0.01\,^2H_{11/2}$
	3	$\Gamma_{4,5}$	43.1	41	$99.91\,^4I_{15/2} + 0.02\,^2H_{11/2} + 0.02\,^4I_{13/2}$
	4	$^2\Gamma_6$	89.1	92	$99.89\,^4I_{15/2} + 0.06\,^4I_{13/2} + 0.02\,^2H_{11/2}$
	5	$\Gamma_{4,5}$	168.3	162	$99.87\,^4I_{15/2} + 0.07\,^4I_{13/2} + 0.02\,^2H_{11/2}$
	6	$^2\Gamma_6$	373.9	376	$99.95\,^4I_{15/2} + 0.02\,^4I_{13/2} + 0.01\,^4F_{9/2}$
	7	$\Gamma_{4,5}$	445.0	—	$99.94\,^4I_{15/2} + 0.04\,^4I_{13/2} + 0.01\,^4I_{11/2}$
	8	$\Gamma_{4,5}$	560.7	—	$99.92\,^4I_{15/2} + 0.06\,^4I_{13/2} + 0.01\,^4F_{9/2}$
$^4I_{13/2}$ (6688)	9	$\Gamma_{4,5}$	6532.0	6530	$99.86\,^4I_{13/2} + 0.04\,^4G_{9/2} + 0.03\,^4I_{9/2}$
	10	$^2\Gamma_6$	6546.8	—	$99.80\,^4I_{13/2} + 0.07\,^4I_{11/2} + 0.03\,^4I_{15/2}$
	11	$\Gamma_{4,5}$	6571.3	6564	$99.71\,^4I_{13/2} + 0.17\,^4I_{11/2} + 0.04\,^4I_{9/2}$
	12	$\Gamma_{4,5}$	6619.0	6627	$99.51\,^4I_{13/2} + 0.41\,^4I_{11/2} + 0.02\,^4I_{9/2}$
	13	$\Gamma_{4,5}$	6779.6	6773	$99.80\,^4I_{13/2} + 0.12\,^4I_{15/2} + 0.03\,^4I_{11/2}$
	14	$^2\Gamma_6$	6802.0	6806	$99.64\,^4I_{13/2} + 0.19\,^4I_{11/2} + 0.11\,^4I_{15/2}$
	15	$\Gamma_{4,5}$	6885.3	—	$99.76\,^4I_{13/2} + 0.17\,^4I_{11/2} + 0.05\,^4I_{15/2}$
$^4I_{11/2}$ (10321)	16	$\Gamma_{4,5}$	10211.3	10211	$99.78\,^4I_{11/2} + 0.05\,^2G_{7/2} + 0.04\,^4I_{13/2}$
	17	$^2\Gamma_6$	10230.1	10230	$99.68\,^4I_{11/2} + 0.11\,^4F_{9/2} + 0.08\,^4I_{9/2}$
	18	$\Gamma_{4,5}$	10268.6	10270	$99.74\,^4I_{11/2} + 0.08\,^4F_{9/2} + 0.08\,^4I_{9/2}$
	19	$\Gamma_{4,5}$	10352.8	10349	$99.29\,^4I_{11/2} + 0.38\,^4I_{13/2} + 0.24\,^4F_{9/2}$
	20	$\Gamma_{4,5}$	10399.5	—	$99.57\,^4I_{11/2} + 0.34\,^4I_{13/2} + 0.03\,^4I_{9/2}$
	21	$^2\Gamma_6$	10422.6	10424	$99.42\,^4I_{11/2} + 0.31\,^4I_{9/2} + 0.20\,^4I_{13/2}$
$^4I_{9/2}$ (12600)	22	$^2\Gamma_6$	12403.0	12399	$99.60\,^4I_{9/2} + 0.17\,^4I_{11/2} + 0.14\,^4F_{9/2}$
	23	$\Gamma_{4,5}$	12500.0	12508	$99.59\,^4I_{9/2} + 0.08\,^4I_{11/2} + 0.07\,^4S_{3/2}$
	24	$\Gamma_{4,5}$	12622.4	12626	$99.70\,^4I_{9/2} + 0.09\,^4F_{9/2} + 0.06\,^4I_{11/2}$
	25	$^2\Gamma_6$	12646.9	12645	$99.42\,^4I_{9/2} + 0.23\,^4F_{9/2} + 0.21\,^4I_{11/2}$
	26	$\Gamma_{4,5}$	12779.8	—	$99.63\,^4I_{9/2} + 0.13\,^4F_{9/2} + 0.10\,^2H_{11/2}$
$^4F_{9/2}$ (15335)	27	$^2\Gamma_6$	15142.4	15149	$99.45\,^4F_{9/2} + 0.26\,^4I_{9/2} + 0.13\,^2H_{11/2}$
	28	$\Gamma_{4,5}$	15296.8	15298	$99.46\,^4F_{9/2} + 0.16\,^2H_{11/2} + 0.15\,^4I_{9/2}$
	29	$\Gamma_{4,5}$	15369.1	—	$99.41\,^4F_{9/2} + 0.17\,^4I_{11/2} + 0.13\,^2H_{11/2}$
	30	$^2\Gamma_6$	15406.2	15402	$99.58\,^4F_{9/2} + 0.14\,^2H_{11/2} + 0.09\,^4I_{9/2}$
	31	$\Gamma_{4,5}$	15446.0	15440	$99.48\,^4F_{9/2} + 0.22\,^2H_{11/2} + 0.13\,^4I_{11/2}$
$^4S_{3/2}$ (18411)	32	$^2\Gamma_6$	18305.2	18307	$96.46\,^4S_{3/2} + 3.37\,^2H_{11/2} + 0.03\,^4I_{9/2}$
	33	$\Gamma_{4,5}$	18445.8	18442	$94.03\,^4S_{3/2} + 5.70\,^2H_{11/2} + 0.08\,^4I_{9/2}$
$^2H_{11/2}$ (19094)	34	$\Gamma_{4,5}$	19009.8	19013	$97.44\,^2H_{11/2} + 1.24\,^4S_{3/2} + 0.74\,^4F_{7/2}$
	35	$\Gamma_{4,5}$	19041.7	19048	$97.66\,^2H_{11/2} + 1.26\,^4S_{3/2} + 0.64\,^4F_{7/2}$
	36	$^2\Gamma_6$	19085.4	19082	$97.45\,^2H_{11/2} + 1.35\,^4S_{3/2} + 0.83\,^4F_{7/2}$
	37	$^2\Gamma_6$	19115.2	19106	$96.85\,^2H_{11/2} + 1.98\,^4S_{3/2} + 0.86\,^4F_{7/2}$
	38	$\Gamma_{4,5}$	19148.8	19144	$99.25\,^2H_{11/2} + 0.38\,^4S_{3/2} + 0.25\,^4F_{7/2}$
	39	$\Gamma_{4,5}$	19186.3	19207	$96.06\,^2H_{11/2} + 2.85\,^4S_{3/2} + 0.80\,^4F_{7/2}$
$^4F_{7/2}$ (20458)	40	$\Gamma_{4,5}$	20290.8	20285	$98.85\,^4F_{7/2} + 0.55\,^2H_{11/2} + 0.17\,^4F_{5/2}$
	41	$\Gamma_{4,5}$	20422.1	20422	$97.33\,^4F_{7/2} + 1.39\,^2H_{11/2} + 1.04\,^4F_{5/2}$
	42	$^2\Gamma_6$	20489.2	20492	$97.79\,^4F_{7/2} + 1.66\,^2H_{11/2} + 0.24\,^4F_{3/2}$
	43	$\Gamma_{4,5}$	20629.6	20630	$98.93\,^4F_{7/2} + 0.46\,^2H_{11/2} + 0.34\,^4F_{5/2}$
$^4F_{5/2}$ (22191)	44	$^2\Gamma_6$	22118.3	22117	$87.34\,^4F_{5/2} + 12.28\,^4F_{3/2} + 0.09\,^2G_{7/2}$
	45	$\Gamma_{4,5}$	22163.1	22164	$97.89\,^4F_{5/2} + 1.27\,^4F_{7/2} + 0.28\,^2H_{11/2}$
	46	$\Gamma_{4,5}$	22249.5	22251	$99.23\,^4F_{5/2} + 0.20\,^4F_{7/2} + 0.16\,^4G_{9/2}$

Table 4 (cont'd). Experimental and best fit theoretical energy levels of Er^{3+} in C_3 site in $Ca_5(PO_4)_3F$.[a]

$^{2S+1}L_J$ centroids (cm^{-1})[b]	Level	Γ_n	Energy (cm^{-1}) Theor.	Expt	Free-ion mixture (%)
$^4F_{3/2}$	47	$^2\Gamma_6$	22593.9	—	$87.09\,^4F_{3/2} + 12.25\,^4F_{5/2} + 0.25\,^4G_{9/2}$
(22639)	48	$\Gamma_{4,5}$	22741.7	22742	$99.35\,^4F_{3/2} + 0.26\,^4F_{5/2} + 0.13\,^2G_{7/2}$
$^2G_{9/2}$	49	$^2\Gamma_6$	24451.7	24448	$99.33\,^2G_{9/2} + 0.45\,^2K_{15/2} + 0.07\,^4G_{11/2}$
(24651)	50	$\Gamma_{4,5}$	24568.0	24575	$97.92\,^2G_{9/2} + 1.53\,^4G_{11/2} + 0.38\,^2K_{15/2}$
	51	$^2\Gamma_6$	24678.3	24678	$98.83\,^2G_{9/2} + 0.71\,^4G_{11/2} + 0.22\,^2K_{15/2}$
	52	$\Gamma_{4,5}$	24693.9	24695	$98.73\,^2G_{9/2} + 0.84\,^4G_{11/2} + 0.20\,^2K_{15/2}$
	53	$\Gamma_{4,5}$	24764.6	—	$97.80\,^2G_{9/2} + 1.46\,^4G_{11/2} + 0.50\,^2K_{15/2}$
$^4G_{11/2}$	54	$\Gamma_{4,5}$	26261.1	26261	$96.99\,^4G_{11/2} + 1.86\,^2G_{9/2} + 0.55\,^2K_{15/2}$
(26367)	55	$^2\Gamma_6$	26272.9	26278	$98.56\,^4G_{11/2} + 0.90\,^4G_{9/2} + 0.37\,^2K_{15/2}$
	56	$\Gamma_{4,5}$	26321.2	26321	$97.03\,^4G_{11/2} + 1.24\,^2G_{9/2} + 1.02\,^2K_{15/2}$
	57	$^2\Gamma_6$	26407.6	26408	$94.90\,^4G_{11/2} + 1.95\,^4G_{9/2} + 1.93\,^2K_{15/2}$
	58	$\Gamma_{4,5}$	26435.9	26425	$97.84\,^4G_{11/2} + 1.24\,^2K_{15/2} + 0.39\,^4G_{9/2}$
	59	$\Gamma_{4,5}$	26478.5	—	$94.47\,^4G_{11/2} + 4.11\,^2K_{15/2} + 0.47\,^4G_{9/2}$
$^4G_{9/2}$	60	$\Gamma_{4,5}$	27352.4	—	$89.44\,^2K_{15/2} + 5.93\,^4G_{11/2} + 3.43\,^4G_{9/2}$
27479[b]	61	$^2\Gamma_6$	27421.7	—	$90.71\,^2K_{15/2} + 4.32\,^4G_{9/2} + 2.71\,^4G_{11/2}$
$^2K_{15/2}$	62	$\Gamma_{4,5}$	27438.4	—	$90.30\,^4G_{9/2} + 4.66\,^2K_{15/2} + 4.56\,^2G_{7/2}$
27800[b]	63	$\Gamma_{4,5}$	27480.8	—	$97.12\,^4G_{9/2} + 1.86\,^2G_{7/2} + 0.50\,^4G_{11/2}$
$^2G_{7/2}$	64	$^2\Gamma_6$	27493.0	—	$86.66\,^4G_{9/2} + 7.05\,^2G_{7/2} + 4.07\,^2K_{15/2}$
27981[a]	65	$\Gamma_{4,5}$	27505.4	—	$95.41\,^4G_{9/2} + 2.35\,^2G_{7/2} + 1.12\,^2K_{15/2}$
	66	$^2\Gamma_6$	27530.3	—	$95.29\,^4G_{9/2} + 3.03\,^2K_{15/2} + 0.80\,^4G_{11/2}$
	67	$\Gamma_{4,5}$	27587.2	—	$96.28\,^2K_{15/2} + 1.96\,^2G_{7/2} + 0.79\,^4G_{9/2}$
	68	$\Gamma_{4,5}$	27807.5	—	$94.16\,^2K_{15/2} + 2.67\,^4G_{9/2} + 2.31\,^2G_{7/2}$
	69	$\Gamma_{4,5}$	27954.2	—	$90.72\,^2G_{7/2} + 7.35\,^2K_{15/2} + 1.72\,^4G_{9/2}$
	70	$^2\Gamma_6$	27982.5	—	$86.97\,^2K_{15/2} + 10.40\,^2G_{7/2} + 2.37\,^4G_{9/2}$
	71	$\Gamma_{4,5}$	28020.8	—	$84.69\,^2G_{7/2} + 13.35\,^2K_{15/2} + 1.40\,^4G_{9/2}$
	72	$\Gamma_{4,5}$	28052.0	—	$90.48\,^2G_{7/2} + 5.06\,^2K_{15/2} + 4.06\,^4G_{9/2}$
	73	$^2\Gamma_6$	28078.5	—	$62.33\,^2K_{15/2} + 33.96\,^2G_{7/2} + 3.52\,^4G_{9/2}$
	74	$^2\Gamma_6$	28105.9	—	$49.83\,^2K_{15/2} + 45.42\,^2G_{7/2} + 4.35\,^4G_{9/2}$
	75	$\Gamma_{4,5}$	28152.2	—	$87.77\,^2K_{15/2} + 11.67\,^2G_{7/2} + 0.28\,^4G_{11/2}$
	76	$\Gamma_{4,5}$	28175.4	—	$92.35\,^2K_{15/2} + 6.99\,^2G_{7/2} + 0.43\,^4G_{9/2}$

With an rms = 4.832 cm^{-1} B_{nm} (cm^{-1}) are $B_{20} = 1281$, $B_{40} = -1600$, $B_{43} = 563$, $B_{60} = -727$, $B_{63} = 505 + i273$, $B_{66} = 87.8 - i279$, and $\text{Im}B_{66} = -277$.

[a]Gruber et al (1994) [10]. The Γ_n labels are from Koster et al (1963) [9].
[b]Aqueous centroids.

Table 5. Experimental and best fit theoretical energy levels of Er^{3+} in C_s site in $Ca_5(PO_4)_3F$.[a]

$^{2S+1}L_J$ centroids (cm^{-1})[b]	Level	Energy (cm^{-1}) Theor.	Expt	Free-ion mixture (%)
$^4I_{15/2}$ (328)	1	5.9	0	$99.90\ ^4I_{15/2} + 0.03\ ^4I_{13/2} + 0.03\ ^2H_{11/2}$
	2	141.5	139	$99.90\ ^4I_{15/2} + 0.05\ ^4I_{13/2} + 0.02\ ^2H_{11/2}$
	3	186.9	194	$99.92\ ^4I_{15/2} + 0.03\ ^4I_{13/2} + 0.02\ ^2H_{11/2}$
	4	257.6	256	$99.92\ ^4I_{15/2} + 0.02\ ^4I_{13/2} + 0.02\ ^4F_{9/2}$
	5	319.6	314	$99.92\ ^4I_{15/2} + 0.04\ ^4I_{13/2} + 0.01\ ^4F_{9/2}$
	6	441.5	—	$99.93\ ^4I_{15/2} + 0.02\ ^4I_{13/2} + 0.01\ ^4F_{9/2}$
	7	522.3	—	$99.91\ ^4I_{15/2} + 0.04\ ^4I_{13/2} + 0.03\ ^4F_{9/2}$
	8	653.7	662	$99.95\ ^4I_{15/2} + 0.03\ ^4I_{13/2} + 0.01\ ^2H_{11/2}$
$^4I_{13/2}$ (6804)	9	6578.8	6583	$99.76\ ^4I_{13/2} + 0.13\ ^4I_{11/2} + 0.03\ ^4G_{9/2}$
	10	6678.0	6667	$99.67\ ^4I_{13/2} + 0.22\ ^4I_{11/2} + 0.03\ ^4G_{9/2}$
	11	6710.5	6713	$99.84\ ^4I_{13/2} + 0.07\ ^4I_{11/2} + 0.03\ ^4I_{15/2}$
	12	6760.5	6773	$99.67\ ^4I_{13/2} + 0.21\ ^4I_{11/2} + 0.05\ ^4I_{15/2}$
	13	6856.6	—	$99.85\ ^4I_{13/2} + 0.04\ ^4I_{15/2} + 0.03\ ^4I_{11/2}$
	14	6906.6	6906	$99.71\ ^4I_{13/2} + 0.17\ ^4I_{11/2} + 0.06\ ^4I_{15/2}$
	15	7045.2	7038	$99.80\ ^4I_{13/2} + 0.10\ ^4I_{11/2} + 0.03\ ^4I_{15/2}$
$^4I_{11/2}$ (10351)	16	10216.4	—	$99.59\ ^4I_{11/2} + 0.15\ ^4I_{13/2} + 0.12\ ^4I_{9/2}$
	17	10279.3	10291	$99.61\ ^4I_{11/2} + 0.18\ ^4I_{9/2} + 0.07\ ^4I_{13/2}$
	18	10308.9	10312	$99.70\ ^4I_{11/2} + 0.11\ ^4I_{13/2} + 0.06\ ^4F_{9/2}$
	19	10359.4	10349	$99.69\ ^4I_{11/2} + 0.15\ ^4I_{13/2} + 0.07\ ^4F_{9/2}$
	20	10399.0	—	$99.54\ ^4I_{11/2} + 0.28\ ^4I_{13/2} + 0.06\ ^4I_{9/2}$
	21	10495.5	10491	$99.57\ ^4I_{11/2} + 0.17\ ^4I_{13/2} + 0.14\ ^4I_{9/2}$
$^4I_{9/2}$ (12605)	22	12431.7	—	$99.66\ ^4I_{9/2} + 0.17\ ^4F_{9/2} + 0.04\ ^4I_{11/2}$
	23	12544.0	12552	$99.63\ ^4I_{9/2} + 0.12\ ^4I_{11/2} + 0.09\ ^4F_{9/2}$
	24	12579.3	12580	$99.50\ ^4I_{9/2} + 0.21\ ^4I_{11/2} + 0.10\ ^4F_{9/2}$
	25	12654.7	12646	$99.49\ ^4I_{9/2} + 0.13\ ^4I_{11/2} + 0.12\ ^4F_{9/2}$
	26	12754.7	—	$99.49\ ^4I_{9/2} + 0.25\ ^4F_{9/2} + 0.10\ ^4I_{11/2}$
$^4F_{9/2}$ (15420)	27	15237.0	15244	$99.18\ ^4F_{9/2} + 0.37\ ^4I_{9/2} + 0.21\ ^2H_{11/2}$
	28	15302.7	15298	$99.45\ ^4F_{9/2} + 0.24\ ^2H_{11/2} + 0.07\ ^4I_{11/2}$
	29	15434.3	15437	$99.34\ ^4F_{9/2} + 0.30\ ^2H_{11/2} + 0.13\ ^4I_{9/2}$
	30	15512.1	15509	$99.45\ ^4F_{9/2} + 0.19\ ^2H_{11/2} + 0.14\ ^4I_{9/2}$
	31	15576.7	15575	$99.71\ ^4F_{9/2} + 0.06\ ^4I_{9/2} + 0.05\ ^2H_{11/2}$
$^4S_{3/2}$ (18432)	32	18300.4	18293	$95.09\ ^4S_{3/2} + 4.61\ ^2H_{11/2} + 0.05\ ^4I_{9/2}$
	33	18448.8	18457	$92.09\ ^4S_{3/2} + 7.54\ ^2H_{11/2} + 0.08\ ^4F_{7/2}$
$^2H_{11/2}$ (19181)	34	19078.3	19087	$97.81\ ^2H_{11/2} + 1.21\ ^4S_{3/2} + 0.72\ ^4F_{7/2}$
	35	19137.2	19141	$97.76\ ^2H_{11/2} + 1.75\ ^4S_{3/2} + 0.21\ ^4F_{7/2}$
	36	19184.2	19179	$97.92\ ^2H_{11/2} + 1.20\ ^4S_{3/2} + 0.29\ ^4F_{7/2}$
	37	19217.0	19198	$93.11\ ^2H_{11/2} + 5.54\ ^4S_{3/2} + 0.89\ ^4F_{7/2}$
	38	19263.1	19259	$97.86\ ^2H_{11/2} + 1.15\ ^4S_{3/2} + 0.54\ ^4F_{7/2}$
	39	19280.4	19295	$97.10\ ^2H_{11/2} + 1.42\ ^4S_{3/2} + 1.03\ ^4F_{7/2}$
$^4F_{7/2}$ (20552)	40	20346.0	20347	$98.36\ ^4F_{7/2} + 0.86\ ^2H_{11/2} + 0.25\ ^4F_{5/2}$
	41	20516.7	20534	$97.59\ ^4F_{7/2} + 1.20\ ^2H_{11/2} + 0.57\ ^4F_{5/2}$
	42	20617.6	20601	$98.18\ ^4F_{7/2} + 0.70\ ^2H_{11/2} + 0.60\ ^4F_{5/2}$
	43	20696.7	20695	$97.93\ ^4F_{7/2} + 0.99\ ^2H_{11/2} + 0.53\ ^4F_{5/2}$
$^4F_{5/2}$ (22204)	44	22125.6	22114	$93.50\ ^4F_{5/2} + 5.47\ ^4F_{3/2} + 0.44\ ^4F_{7/2}$
	45	22162.7	22164	$85.15\ ^4F_{5/2} + 13.08\ ^4F_{3/2} + 1.02\ ^4F_{7/2}$
	46	22245.6	22256	$95.44\ ^4F_{5/2} + 3.48\ ^4F_{3/2} + 0.63\ ^4F_{7/2}$

11

Table 5 (cont'd). Experimental and best fit theoretical energy levels of Er^{3+} in C_s site in $Ca_5(PO_4)_3F$.[a]

$^{2S+1}L_J$ centroids (cm^{-1})[b]	Level	Energy (cm-1)		Free-ion mixture (%)
		Theor.	Expt	
$^4F_{3/2}$ (22599)	47	22551.6	22550	$82.27\,^4F_{3/2} + 16.92\,^4F_{5/2} + 0.37\,^4F_{7/2}$
	48	22740.5	22742	$94.18\,^4F_{3/2} + 5.22\,^4F_{5/2} + 0.16\,^4F_{7/2}$
$^2G_{9/2}$ (24556)	49	24394.2	24401	$98.49\,^2G_{9/2} + 0.70\,^4G_{11/2} + 0.55\,^2K_{15/2}$
	50	24459.9	24448	$98.23\,^2G_{9/2} + 0.93\,^4G_{11/2} + 0.54\,^2K_{15/2}$
	51	24543.5	—	$98.82\,^2G_{9/2} + 0.56\,^4G_{11/2} + 0.37\,^2K_{15/2}$
	52	24582.9	24588	$97.65\,^2G_{9/2} + 1.38\,^4G_{11/2} + 0.61\,^2K_{15/2}$
	53	24673.4	—	$98.20\,^2G_{9/2} + 0.84\,^4G_{11/2} + 0.70\,^2K_{15/2}$
$^4G_{11/2}$ (26398)	54	26214.2	26206	$97.91\,^4G_{11/2} + 1.22\,^4G_{9/2} + 0.54\,^2K_{15/2}$
	55	26261.1	26265	$98.60\,^4G_{11/2} + 0.56\,^4G_{9/2} + 0.38\,^2K_{15/2}$
	56	26369.2	26364	$95.65\,^4G_{11/2} + 1.59\,^2G_{9/2} + 1.33\,^2K_{15/2}$
	57	26465.4	26464	$96.38\,^4G_{11/2} + 1.74\,^4G_{9/2} + 0.97\,^2K_{15/2}$
	58	26520.5	26523	$95.12\,^4G_{11/2} + 1.86\,^4G_{9/2} + 1.67\,^2K_{15/2}$
	59	26560.4	26569	$96.66\,^4G_{11/2} + 1.35\,^2K_{15/2} + 0.82\,^2G_{9/2}$
$^4G_{9/2}$ 27479[b] $^2K_{15/2}$ 27800[b] $^2G_{7/2}$ 27981[b]	60	27293.8	—	$91.95\,^2K_{15/2} + 3.59\,^4G_{9/2} + 1.75\,^4G_{11/2}$
	61	27433.1	—	$82.41\,^4G_{9/2} + 8.44\,^2K_{15/2} + 7.16\,^2G_{7/2}$
	62	27443.6	—	$84.89\,^4G_{9/2} + 7.75\,^2G_{7/2} + 6.53\,^2K_{15/2}$
	63	27474.4	—	$58.33\,^4G_{9/2} + 38.42\,^2K_{15/2} + 1.95\,^2G_{7/2}$
	64	27518.1	—	$77.33\,^4G_{9/2} + 14.88\,^2K_{15/2} + 6.33\,^2G_{7/2}$
	65	27527.1	—	$56.67\,^4G_{9/2} + 37.59\,^2K_{15/2} + 3.31\,^2G_{7/2}$
	66	27559.4	—	$92.19\,^4G_{9/2} + 4.31\,^2K_{15/2} + 1.63\,^4G_{11/2}$
	67	27609.3	—	$89.97\,^2K_{15/2} + 6.58\,^4G_{9/2} + 1.70\,^2G_{7/2}$
	68	27647.8	—	$93.68\,^2K_{15/2} + 2.83\,^4G_{9/2} + 2.11\,^2G_{7/2}$
	69	27830.8	—	$87.20\,^2K_{15/2} + 11.45\,^2G_{7/2} + 0.73\,^4G_{9/2}$
	70	27923.5	—	$90.24\,^2K_{15/2} + 8.26\,^2G_{7/2} + 1.01\,^4G_{9/2}$
	71	27998.8	—	$89.64\,^2G_{7/2} + 5.37\,^2K_{15/2} + 4.62\,^4G_{9/2}$
	72	28043.4	—	$74.37\,^2G_{7/2} + 16.79\,^2K_{15/2} + 8.24\,^4G_{9/2}$
	73	28084.0	—	$82.50\,^2G_{7/2} + 13.36\,^2K_{15/2} + 3.46\,^4G_{9/2}$
	74	28110.4	—	$81.16\,^2G_{7/2} + 10.37\,^2K_{15/2} + 7.81\,^4G_{9/2}$
	75	28209.0	—	$84.17\,^2K_{15/2} + 14.66\,^2G_{7/2} + 0.44\,^2G_{9/2}$
	76	28526.2	—	$97.54\,^2K_{15/2} + 2.10\,^2G_{7/2} + 0.26\,^4G_{11/2}$

The B_{nm} (cm^{-1}) are $B_{20} = 1406$, $B_{22} = 236$, $B_{40} = 744$, $B_{42} = -1306 - i587$, $\mathrm{Im}B_{42} = 50.5 + i566$, $B_{60} = -42$, $B_{62} = 203 - i225$, $B_{64} = 397 + i165$, and $B_{66} = -131 + i123$. The rms = 7.892 cm^{-1}.

[a]Gruber et al (1994) [10]. All levels are the $\Gamma_3 + \Gamma_4$ Kramers doublets in the notation of Koster et al (1963) [9].

Table 6. Smoothed crystal-field parameters, B_{nm} (cm^{-1}), for C_3 site in $Ca_5(PO_4)_3F$.

Ion	B_{20}	B_{40}	B_{43}	B_{60}	ReB_{63}	ImB_{63}	ReB_{66}	ImB_{66}
A_{nm}	7509	−3878	1365	−740	514	278	89.4	−284
Ce	1382	−2922	1028	−1801	1251	676	218	−691
Pr	1318	−2507	882	−1388	964	521	168	−533
Nd	1281	−2240	788	−1376	817	442	142	−451
Pm	1261	−2070	729	−1052	731	395	127	−404
Sm	1252	−1958	689	−977	679	367	118	−375
Eu	1251	−1875	660	−925	643	347	112	−355
Gd	1252	−1806	635	−878	610	330	106	−337
Tb	1256	−1741	613	−831	577	312	100	−319
Dy	1262	−1683	592	−785	545	295	94.8	−301
Ho	1270	−1635	575	−749	520	281	90.4	−287
Er	1281	−1600	563	−727	505	273	87.8	−279
Tm	1293	−1572	553	−714	496	268	86.2	−274
Yb	1304	−1527	537	−675	469	253	81.5	−259

Table 7. Smoothed crystal-field parameters B_{nm} (cm^{-1}) for C_s site in $Ca_5(PO_4)_3F$.

Ion	B_{20}	B_{22}	B_{40}	ReB_{42}	ImB_{42}	ReB_{44}	ImB_{44}
A_{nm}	8242	1383	1803	−3165	−1423	122	1372
Ce	1517	255	1359	−2385	−1072	92.2	1034
Pr	1447	243	1166	−2046	−920	79.1	887
Nd	1406	236	1342	−1828	−822	70.7	792
Pm	1384	232	963	−1690	−760	65.3	732
Sm	1375	231	910	−1598	−718	61.8	693
Eu	1373	230	872	−1531	−688	59.2	663
Gd	1375	231	840	−1474	−662	57.0	639
Tb	1379	231	810	−1421	−639	55.0	616
Dy	1385	233	783	−1374	−618	53.1	595
Ho	1394	234	760	−1335	−600	51.6	578
Er	1406	236	744	−1306	−587	50.5	566
Tm	1419	238	731	−1283	−577	49.6	556
Yb	1432	240	710	−1246	−560	48.2	540

Ion	B_{60}	ReB_{62}	ImB_{62}	ReB_{64}	ImB_{64}	ReB_{66}	ImB_{66}
A_{nm}	−42.7	207	−229	404	168	−133	125
Ce	−104	503	−557	983	409	−325	305
Pr	−80.2	387	−429	758	315	−250	235
Nd	−67.9	328	−364	642	267	−212	199
Pm	−60.8	294	−326	574	239	−190	178
Sm	−56.5	273	−302	534	222	−176	165
Eu	−53.4	258	−286	505	210	−167	157
Gd	−50.7	245	−272	480	199	−158	148
Tb	−48.0	232	−257	454	189	−150	141
Dy	−45.4	219	−243	429	178	−142	133
Ho	−43.3	209	−232	409	170	−135	127
Er	−42.0	203	−225	397	165	−131	123
Tm	−41.2	199	−221	390	162	−129	121
Yb	−39.0	188	−209	368	153	−122	114

3. Judd-Ofelt Intensity Parameters

The Judd-Ofelt parameters for the Ca1 (C_3) site and the Ca2 (C_s) site have been calculated and are given in tables 8 and 9, respectively. In the calculation of the Judd-Ofelt parameters, the formula

$$\Omega_t = 28(2t + 1) \sum_k S_k^2 N_k^2(t) , \quad t = 2, 4, \text{ and } 6, \tag{6}$$

from Leavitt and Morrison [11] has been used. The $N_k(t)$ are given there, and

$$S_k^2 = \frac{1}{2k + 1}\left[A_{k0}^2 + 2 \sum_{m=1}^{k} \left| A_{km} \right|^2 \right], \quad k = 1, 3, 5, \text{ and } 7. \tag{7}$$

Table 8. Calculated Judd-Ofelt intensity parameters Ω_k (10^{-20} cm^2) of rare-earth ions in C_3 Ca site in $Ca_5(PO_4)_3F$.[a]

Ion	Ω_2	Ω_4	Ω_6
Ce	22.46	12.95	58.25
Pr	13.61	6.530	24.83
Nd	10.13	4.228	13.63
Pm	8.541	3.253	10.47
Sm	7.769	2.771	8.671
Eu	6.143	2.105	6.131
Gd	4.754	1.575	4.233
Tb	10.06	3.068	10.28
Dy	7.136	2.110	6.376
Ho	5.742	1.648	4.654
Er	5.623	1.567	4.390
Tm	5.583	1.517	4.241
Yb	4.671	1.229	3.231

[a]Hughes et al (1989) [2].

Table 9. Calculated Judd-Ofelt intensity parameters Ω_k (10^{-20} cm^2) of rare-earth ions in C_s site in $Ca_5(PO_4)_3F$.[a]

Ion	Ω_2	Ω_4	Ω_6
Ce	13.89	18.60	46.88
Pr	8.19	9.373	20.03
Nd	6.68	6.162	11.00
Pm	4.983	4.792	8.450
Sm	4.456	4.041	6.990
Eu	3.525	3.030	4.954
Gd	2.737	2.230	3.426
Tb	5.498	4.772	8.228
Dy	3.936	3.204	5.118
Ho	3.180	2.472	3.739
Er	3.096	2.364	3.525
Tm	3.058	2.304	3.0402
Yb	2.563	1.852	2.594

[a]Hughes et al (1989) [2].

4. Predicted Energy Levels for Ca1 Site (C_3) and Ca2 Site (C_s)

The smoothed crystal-field parameters for the Ca1 site given in table 6 have been used in the calculation of the energy levels of the entire triply ionized rare-earth series Ce^{3+} through Yb^{3+}; these energy levels are given in tables 6 through 23. The smoothed crystal-field parameters for the Ca2 site given in table 7 have been used for a similar calculation, with the results given in tables 24 through 35. The g values for those ions having doublet ground states have been calculated and are given in table 10.

Table 10. Predicted g values of ground state of triply ionized rare-earth ions in two Ca sites in $Ca_5(PO_4)_3F$.

Ion	C_3		$C_s{}^a$		
	$g\parallel$	$g\perp$	$g\parallel$	$g\perp1^b$	$g\perp2^b$
Ce	−3.6897	0.317	2.467	1.629	0.326
Pr^c	—	—	—	—	—
Nd	4.556	0.930	2.210	3.660	0.934
Pm	1.544	0	—	—	—
Sm	1.079	0.255	−0.345	0.736	0.134
Eu^c	—	—	—	—	—
Gd	1.994	7.979	0.931	12.845	1.857
Tb^c	—	—	—	—	—
Dy	−14.422	0.276	−19.487	0.011	0.007
Ho	16.537	0	—	—	—
Er	0.694	8.737	−0.532	16.159	1.027
Tm^c	—	—	—	—	—
Yb	6.645	—	−0.012	7.056	0.097

^{a}In C_s symmetry, g values exist only for rare-earth elements with an odd number of f electrons.

$^b g\perp1$ and $g\perp2$ are magnitudes of principal g factors in a, b plane ($g\parallel$ is parallel to c-axis).

^{c}These ions have singlet ground states in C_3 sites as well as C_s sites.

Table 11. Splitting (cm^{-1}) of ^4I_J ($J = 15/2$ to 9/2) for Er^{3+} in $Ca_5(PO_4)_3F$, LaF_3, Y_2O_3.

State	$Ca_5(PO_4)_3F$		$LaF_3{}^b$	$Y_2O_3{}^c$
	$C_3{}^a$	$C_s{}^a$		
$^4I_{15/2}$	562	662	443	510
$^4I_{13/2}$	353	455	219	357
$^4I_{11/2}$	212	280	94	186
$^4I_{9/2}$	377	323	311	280

^{a}This work, table 5, for C_3 site and table 6 for C_s site.
^{b}Morrison and Leavitt (1979) [5].
^{c}Chang et al (1982) [8] (C_2 site).

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
				Table 12. Predicted energy levels for Ce^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_3$ site. B$_{nm}$ from table 6.
1	$\Gamma_{4,5}$	$^2F_{5/2}$	0	$97.52\,^2F_{5/2} + 2.48\,^2F_{7/2}$
2	$\Gamma_{4,5}$	250	573.8	$93.34\,^2F_{5/2} + 6.66\,^2F_{7/2}$
3	$^2\Gamma_6$	—	1074.1	$96.86\,^2F_{5/2} + 3.14\,^2F_{7/2}$
4	$\Gamma_{4,5}$	$^2F_{7/2}$	2272.0	$97.75\,^2F_{7/2} + 2.25\,^2F_{5/2}$
5	$\Gamma_{4,5}$	2550	2771.5	$97.60\,^2F_{7/2} + 2.40\,^2F_{5/2}$
6	$^2\Gamma_6$	—	3532.0	$96.86\,^2F_{7/2} + 3.14\,^2F_{5/2}$
7	$\Gamma_{4,5}$	—	3559.9	$95.51\,^2F_{7/2} + 49\,^2F_{5/2}$

[a]Irreducible representations of C$_3$ double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.
[b]Aqueous centroids (cm^{-1}).

Table 13. Predicted energy levels for Pr^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_3$ site. B$_{nm}$ from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^3H_4$	0	$98.44\,^3H_4 + 0.69\,^3F_3 + 0.63\,^3H_5$
2	$\Gamma_{2,3}$	245	109	$96.47\,^3H_4 + 2.05\,^3H_5 + 1.15\,^3F_2$
3	Γ_1		167	$99.25\,^3H_4 + 0.23\,^3F_3 + 0.19\,3F\,4$
4	$\Gamma_{2,3}$		254	$98.26\,^3H_4 + 1.17\,^3H_5 + 0.24\,^3F_2$
5	$\Gamma_{2,3}$		739	$95.94\,^3H_4 + 3.59\,^3H_5 + 0.25\,^3F_2$
6	Γ_1		1114	$98.45\,^3H_4 + 0.86\,^3H_5 + 0.45\,^3F_3$
7	$\Gamma_{2,3}$	$^3H_5$	2193	$96.77\,^3H_5 + 1.24\,^3H_4 + 0.69\,^3H_6$
8	Γ_1	2323	2200	$97.50\,^3H_5 + 1.07\,^3F_3 + 0.57\,^3H_4$
9	Γ_1		2258	$95.80\,^3H_5 + 1.88\,^3H_6 + 1.10\,^3F_3$
10	$\Gamma_{2,3}$		2289	$98.23\,^3H_5 + 0.69\,^3H_6 + 0.33\,^3F_2$
11	$\Gamma_{2,3}$		2509	$92.33\,^3H_5 + 3.00\,^3H_6 + 2.63\,^3H_4$
12	$\Gamma_{2,3}$		2928	$93.88\,^3H_5 + 2.97\,^3H_4 + 1.58\,^3H_6$
13	Γ_1		3089	$98.55\,^3H_5 + 0.89\,^3H_6 + 0.25\,^3F_3$
14	$\Gamma_{2,3}$	$^3H_6$	4184	$93.75\,^3H_6 + 3.10\,^3F_4 + 1.58\,^3H_5$
15	Γ_1	4496	4230	$95.23\,^3H_6 + 1.61\,^3F_3 + 1.55\,^3H_5$
16	Γ_1		4354	$96.64\,^3H_6 + 1.51\,^3F_2 + 1.19\,^3F_4$
17	$\Gamma_{2,3}$		4441	$96.23\,^3H_6 + 2.05\,^3F_2 + 0.98\,^3F_3$
18	Γ_1		4533	$96.29\,^3H_6 + 1.61\,^3H_5 + 1.51\,^3F_3$
19	Γ_1		4578	$96.48\,^3H_6 + 1.89\,^3F_3 + 1.05\,^3H_5$
20	$\Gamma_{2,3}$		4894	$88.71\,^3H_6 + 7.40\,^3F_2 + 3.29\,^3H_5$
21	$\Gamma_{2,3}$		5196	$83.31\,^3H_6 + 13.85\,^3F_2 + 1.37\,^3F_4$
22	Γ_1	$^3F_2$	5256	$60.34\,^3F_2 + 37.03\,^3H_6 + 1.49\,^3F_4$
23	$\Gamma_{2,3}$	5149	5337	$87.55\,^3F_2 + 10.60\,^3H_6 + 0.88\,^3H_5$
24	Γ_1	$^3F_3$	5396	$58.13\,^3H_6 + 36.57\,^3F_2 + 4.03\,^3F_3$
25	$\Gamma_{2,3}$	6540	5680	$78.14\,^3F_2 + 11.21\,^3H_6 + 6.58\,^3F_3$
26	Γ_1	$^3F_4$	6611	$89.27\,^3F_3 + 9.76\,^3F_4 + 0.83\,^3H_6$
27	$\Gamma_{2,3}$	6973	6725	$92.97\,^3F_3 + 3.17\,^3F_4 + 1.99\,^3F_2$
28	Γ_1		6762	$69.01\,^3F_4 + 27.32\,^3F_3 + 1.44\,^1G_4$
29	Γ_1		6819	$54.19\,^3F_3 + 43.19\,^3F_4 + 1.58\,^3H_6$
30	$\Gamma_{2,3}$		6868	$92.78\,^3F_3 + 2.46\,^3H_6 + 2.24\,^3F_2$
31	$\Gamma_{2,3}$		7135	$97.90\,^3F_4 + 0.65\,^3H_6 + 0.48\,^3F_2$
32	Γ_1		7189	$68.99\,^3F_4 + 26.80\,^3F_3 + 2.67\,^3H_6$
33	$\Gamma_{2,3}$		7219	$95.78\,^3F_4 + 2.48\,^3F_3 + 0.93\,^3H_6$
34	Γ_1		7249	$55.00\,^3F_3 + 39.15\,^3F_4 + 3.40\,^3H_6$
35	Γ_1		7408	$58.80\,^3F_4 + 32.86\,^3F_3 + 5.56\,^3H_6$
36	$\Gamma_{2,3}$		7619	$93.02\,^3F_4 + 4.11\,^3H_6 + 1.07\,^3F_3$

Table 13 (cont'd). Predicted energy levels for Pr^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
37	Γ_1	$^1G_4$	9560	$95.75\ ^1G_4 + 3.09\ ^3F_4 + 0.56\ ^3H_6$
38	Γ_1	9885	9723	$97.92\ ^1G_4 + 1.11\ ^3F_4 + 0.50\ ^3H_6$
39	$\Gamma_{2,3}$		10039	$98.87\ ^1G_4 + 0.43\ ^3F_4 + 0.30\ ^3H_6$
40	$\Gamma_{2,3}$		10103	$99.33\ ^1G_4 + 0.14\ ^3H_6 + 0.13\ ^1I_6$
41	Γ_1		10223	$99.42\ ^1G_4 + 0.18\ ^1I_6 + 0.13\ ^3F_4$
42	$\Gamma_{2,3}$		10645	$98.71\ ^1G_4 + 0.53\ ^3F_4 + 0.32\ ^3H_6$
43	Γ_1	$^1D_2$	16328	$98.12\ ^1D_2 + 1.52\ ^1I_6 + 0.16\ ^3P_2$
44	$\Gamma_{2,3}$	16840	17079	$99.18\ ^1D_2 + 0.51\ ^1I_6 + 0.09\ ^1G_4$
45	$\Gamma_{2,3}$		17323	$98.31\ ^1D_2 + 1.36\ ^1I_6 + 0.14\ ^1G_4$
46	Γ_1	$^3P_0$	20425	$99.97\ ^1I_6 + 0.02\ ^1G_4$
47	Γ_1	20706	20444	$99.33\ ^1I_6 + 0.52\ ^1D_2 + 0.11\ ^3P_2$
48	Γ_1	$^3P_1$	20897	$94.80\ ^3P_0 + 4.34\ ^3P_2 + 0.52\ ^1I_6$
49	$\Gamma_{2,3}$	21330	21384	$90.11\ ^3P_1 + 6.45\ ^3P_2 + 2.95\ ^1I_6$
50	$\Gamma_{2,3}$	$^1I_6$	21490	$97.05\ ^1I_6 + 2.60\ ^3P_1 + 0.20\ ^1D_2$
51	Γ_1	21500	21789	$96.46\ ^1I_6 + 1.88\ ^3P_2 + 0.68\ ^3P_0$
52	$\Gamma_{2,3}$		21810	$99.17\ ^1I_6 + 0.37\ ^3P_2 + 0.31\ ^1D_2$
53	Γ_1		21837	$99.87\ ^3P_1 + 0.07\ ^3H_5 + 0.03\ ^1I_6$
54	$\Gamma_{2,3}$		22168	$97.74\ ^1I_6 + 1.30\ ^3P_2 + 0.45\ ^1D_2$
55	$\Gamma_{2,3}$		22265	$92.16\ ^1I_6 + 5.80\ ^3P_2 + 1.12\ ^3P_1$
56	Γ_1		22270	$98.27\ ^1I_6 + 1.10\ ^3P_2 + 0.24\ ^1G_4$
57	Γ_1		22354	$83.70\ ^1I_6 + 14.27\ ^3P_2 + 1.35\ ^3P_0$
58	Γ_1	$^3P_2$	22622	$77.80\ ^3P_2 + 19.24\ ^1I_6 + 2.67\ ^3P_0$
59	$\Gamma_{2,3}$	22535	22840	$87.98\ ^3P_2 + 6.46\ ^1I_6 + 5.20\ ^3P1$
60	$\Gamma_{2,3}$		23056	$97.62\ ^3P_2 + 2.10\ ^1I_6 + 0.11\ ^3P_1$
61	Γ_1	$^1S_0$ 46901	47169	$99.86\ ^1S_0 + 0.06\ ^1I_6 + 0.03\ ^1D_2$

[a]Irreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.
[b]Aqueous centroids (cm^{-1}).

Table 14. Predicted energy levels for Nd^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	$\Gamma_{4,5}$	$^4I_{9/2}$	0	$98.44\ ^4I_{9/2} + 1.38\ ^4I_{11/2} + 0.13\ ^4I_{13/2}$
2	$^2\Gamma_6$	130	25	$97.83\ ^4I_{9/2} + 1.80\ ^4I_{11/2} + 0.28\ ^4I_{13/2}$
3	$\Gamma_{4,5}$		335	$97.23\ ^4I_{9/2} + 2.62\ ^4I_{11/2} + 0.05\ ^4G_{5/2}$
4	$\Gamma_{4,5}$		530	$99.12\ ^4I_{9/2} + 0.53\ ^4I_{11/2} + 0.17\ ^4I_{13/2}$
5	$^2\Gamma_6$		658	$97.75\ ^4I_{9/2} + 2.06\ ^4I_{11/2} + 0.08\ ^4I_{13/2}$
6	$^2\Gamma_6$	$^4I_{11/2}$	2060	$96.95\ ^4I_{11/2} + 1.58\ ^4I_{9/2} + 1.34\ ^4I_{13/2}$
7	$\Gamma_{4,5}$	2006	2142	$97.09\ ^4I_{11/2} + 2.34\ ^4I_{13/2} + 0.24\ ^4I_{9/2}$
8	$\Gamma_{4,5}$		2174	$95.48\ ^4I_{11/2} + 2.22\ ^4I_{9/2} + 2.16\ ^4I_{13/2}$
9	$\Gamma_{4,5}$		2376	$97.27\ ^4I_{11/2} + 1.59\ ^4I_{9/2} + 1.03\ ^4I_{13/2}$
10	$\Gamma_{4,5}$		2403	$98.94\ ^4I_{11/2} + 0.41\ ^4I_{9/2} + 0.33\ ^4I_{13/2}$
11	$^2\Gamma_6$		2415	$96.68\ ^4I_{11/2} + 2.28\ ^4I_{9/2} + 0.86\ ^4I_{13/2}$
12	$\Gamma_{4,5}$	$^4I_{13/2}$	4015	$97.45\ ^4I_{13/2} + 1.49\ ^4I_{11/2} + 0.98\ ^4I_{15/2}$
13	$^2\Gamma_6$	4004	4104	$96.39\ ^4I_{13/2} + 1.79\ ^4I_{15/2} + 1.51\ ^4I_{11/2}$
14	$\Gamma_{4,5}$		4121	$96.90\ ^4I_{13/2} + 2.48\ ^4I_{15/2} + 0.46\ ^4I_{11/2}$
15	$\Gamma_{4,5}$		4385	$97.53\ ^4I_{13/2} + 1.58\ ^4I_{11/2} + 0.55\ ^4I_{15/2}$
16	$^2\Gamma_6$		4404	$98.04\ ^4I_{13/2} + 0.98\ ^4I_{15/2} + 0.68\ ^4I_{11/2}$
17	$\Gamma_{4,5}$		4408	$97.64\ ^4I_{13/2} + 1.06\ ^4I_{15/2} + 1.05\ ^4I_{11/2}$
18	$\Gamma_{4,5}$		4436	$98.01\ ^4I_{13/2} + 1.18\ ^4I_{11/2} + 0.68\ ^4I_{15/2}$

Table 14 (cont'd). Predicted energy levels for Nd^{3+} in Ca$_5$(PO$_4$)$_3$F, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
19	$\Gamma_{4,5}$	$^4I_{15/2}$	5890	$97.87\ ^4I_{15/2} + 1.99\ ^4I_{13/2} + 0.04\ ^4F_{9/2}$
20	$\Gamma_{4,5}$	6080	6059	$98.64\ ^4I_{15/2} + 1.10\ ^4I_{13/2} + 0.17\ ^4I_{11/2}$
21	$^2\Gamma_6$		6144	$99.01\ ^4I_{15/2} + 0.83\ ^4I_{13/2} + 0.04\ ^4F_{9/2}$
22	$\Gamma_{4,5}$		6377	$98.63\ ^4I_{15/2} + 1.08\ ^4I_{13/2} + 0.11\ ^4I_{11/2}$
23	$^2\Gamma_6$		6497	$99.25\ ^4I_{15/2} + 0.39\ ^4I_{13/2} + 0.09\ ^4F_{9/2}$
24	$\Gamma_{4,5}$		6544	$99.04\ ^4I_{15/2} + 0.52\ ^4I_{13/2} + 0.13\ ^4F_{9/2}$
25	$\Gamma_{4,5}$		6675	$98.67\ ^4I_{15/2} + 1.02\ ^4I_{13/2} + 0.08\ ^4F_{9/2}$
26	$^2\Gamma_6$		6732	$98.32\ ^4I_{15/2} + 1.51\ ^4I_{13/2} + 0.06\ ^4I_{11/2}$
27	$\Gamma_{4,5}$	$^4F_{3/2}$	11678	$97.83\ ^4F_{3/2} + 0.63\ ^4F_{5/2} + 0.56\ ^2H_{9/2}$
28	$^2\Gamma_6$	11526	11826	$94.37\ ^4F_{3/2} + 3.69\ ^4F_{5/2} + 0.93\ ^4F_{7/2}$
29	$\Gamma_{4,5}$	$^4F_{5/2}$	12670	$86.44\ ^4F_{5/2} + 11.44\ ^2H_{9/2} + 1.02\ ^4F_{7/2}$
30	$\Gamma_{4,5}$	12573	12800	$56.77\ ^4F_{5/2} + 37.86\ ^2H_{9/2} + 4.03\ ^4F_{7/2}$
31	$^2\Gamma_6$	$^2H_{9/2}$	12831	$87.91\ ^2H_{9/2} + 9.92\ ^4F_{5/2} + 0.98\ ^4F_{3/2}$
32	$\Gamma_{4,5}$	12738	12912	$63.42\ ^2H_{9/2} + 34.89\ ^4F_{5/2} + 0.95\ ^4F_{7/2}$
33	$^2\Gamma_6$		12943	$83.94\ ^4F_{5/2} + 12.03\ ^2H_{9/2} + 3.30\ ^4F_{3/2}$
34	$\Gamma_{4,5}$		13039	$85.76\ ^2H_{9/2} + 12.40\ ^4F_{5/2} + 1.17\ ^4F_{7/2}$
35	$^2\Gamma_6$		13147	$98.06\ ^2H_{9/2} + 1.29\ ^4F_{5/2} + 0.23\ ^4F_{9/2}$
36	$\Gamma_{4,5}$		13174	$98.22\ ^2H_{9/2} + 0.87\ ^4F_{7/2} + 0.40\ ^4F_{5/2}$
37	$\Gamma_{4,5}$		13657	$92.59\ ^4F_{7/2} + 2.80\ ^4F_{5/2} + 1.79\ ^4S_{3/2}$
38	$\Gamma_{4,5}$	$^4S_{3/2}$	13711	$96.19\ ^4S_{3/2} + 2.60\ ^4F_{7/2} + 0.43\ ^4G_{5/2}$
39	$^2\Gamma_6$	13459	13737	$94.92\ ^4S_{3/2} + 4.12\ ^4F_{7/2} + 0.20\ ^4G_{5/2}$
40	$^2\Gamma_6$	$^4F_{7/2}$	13872	$92.28\ ^4F_{7/2} + 4.33\ ^4S_{3/2} + 0.93\ ^2H_{9/2}$
41	$\Gamma_{4,5}$	13564	13884	$95.10\ ^4F_{7/2} + 2.24\ ^4F_{5/2} + 1.12\ ^4F_{9/2}$
42	$\Gamma_{4,5}$		13982	$94.68\ ^4F_{7/2} + 3.29\ ^4F_{9/2} + 1.23\ ^4F_{5/2}$
43	$\Gamma_{4,5}$	$^4F_{9/2}$	15018	$97.36\ ^4F_{9/2} + 0.89\ ^2H_{11/2} + 0.53\ ^4F_{7/2}$
44	$\Gamma_{4,5}$	14854	15082	$95.39\ ^4F_{9/2} + 3.08\ ^4F_{7/2} + 0.71\ ^2H_{11/2}$
45	$^2\Gamma_6$		15086	$98.04\ ^4F_{9/2} + 0.71\ ^4F_{7/2} + 0.41\ ^2H_{11/2}$
46	$\Gamma_{4,5}$		15166	$97.49\ ^4F_{9/2} + 1.46\ ^4F_{7/2} + 0.32\ ^2G_{7/2}$
47	$^2\Gamma_6$		15380	$99.07\ ^4F_{9/2} + 0.31\ ^2G_{7/2} + 0.21\ ^2H_{9/2}$
48	$\Gamma_{4,5}$	$^2H_{11/2}$	16263	$98.22\ ^2H_{11/2} + 1.15\ ^2G_{7/2} + 0.15\ ^4F_{7/2}$
49	$^2\Gamma_6$	16043	16282	$98.78\ ^2H_{11/2} + 0.81\ ^2G_{7/2} + 0.11\ ^4F_{9/2}$
50	$\Gamma_{4,5}$		16308	$97.59\ ^2H_{11/2} + 1.76\ ^2G_{7/2} + 0.33\ ^4F_{9/2}$
51	$^2\Gamma_6$		16319	$98.63\ ^2H_{11/2} + 0.50\ ^2G_{7/2} + 0.46\ ^4F_{9/2}$
52	$\Gamma_{4,5}$		16350	$98.30\ ^2H_{11/2} + 0.88\ ^4F_{9/2} + 0.33\ ^2H_{9/2}$
53	$\Gamma_{4,5}$		16404	$98.99\ ^2H_{11/2} + 0.46\ ^4F_{9/2} + 0.35\ ^2G_{7/2}$
54	$\Gamma_{4,5}$	$^4G_{5/2}$	17215	$83.80\ ^4G_{5/2} + 14.59\ ^2G_{7/2} + 0.37\ ^2H_{11/2}$
55	$\Gamma_{4,5}$	17167	17379	$73.71\ ^4G_{5/2} + 25.12\ ^2G_{7/2} + 0.50\ ^2H_{11/2}$
56	$^2\Gamma_6$	$^2G_{7/2}$	17490	$64.48\ ^2G_{7/2} + 33.67\ ^4G_{5/2} + 0.96\ ^2H_{11/2}$
57	$\Gamma_{4,5}$	17334	17674	$96.68\ ^2G_{7/2} + 1.56\ ^4G_{5/2} + 1.06\ ^2H_{11/2}$
58	$\Gamma_{4,5}$		17734	$84.89\ ^2G_{7/2} + 13.79\ ^4G_{5/2} + 0.51\ ^2H_{11/2}$
59	$\Gamma_{4,5}$		17799	$72.81\ ^2G_{7/2} + 24.91\ ^4G_{5/2} + 1.10\ ^2H_{11/2}$
60	$^2\Gamma_6$		17815	$65.04\ ^4G_{5/2} + 33.45\ ^2G_{7/2} + 0.49\ ^2H_{11/2}$

[a]Irreducible representations of C_3 double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.
[b]Aqueous centroids (cm^{-1}).

Table 15. Predicted energy levels for Pm^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	$\Gamma_{2,3}$	$^5I_4$	0	$98.57\ ^5I_4 + 1.14\ ^5I_5 + 0.22\ ^5I_6$
2	Γ_1	99	122	$99.19\ ^5I_4 + 0.63\ ^5I_5 + 0.08\ ^5I_6$
3	$\Gamma_{2,3}$		143	$96.77\ ^5I_4 + 2.88\ ^5I_5 + 0.27\ ^5I_6$
4	$\Gamma_{2,3}$		320	$97.47\ ^5I_4 + 1.86\ ^5I_5 + 0.57\ ^5I_6$
5	Γ_1		368	$93.90\ ^5I_4 + 5.70\ ^5I_5 + 0.30\ ^5I_6$
6	Γ_1		547	$97.57\ ^5I_4 + 1.82\ ^5I_5 + 0.54\ ^5I_6$
7	Γ_1	$^5I_5$	1533	$99.55\ ^5I_5 + 0.14\ ^5I_6 + 0.10\ ^5I_7$
8	$\Gamma_{2,3}$	1577	1621	$97.20\ ^5I_5 + 1.90\ ^5I_4 + 0.76\ ^5I_6$
9	$\Gamma_{2,3}$		1710	$98.59\ ^5I_5 + 0.60\ ^5I_6 + 0.46\ ^5I_7$
10	$\Gamma_{2,3}$		1803	$96.94\ ^5I_5 + 1.81\ ^5I_6 + 0.86\ ^5I_4$
11	Γ_1		1814	$94.12\ ^5I_5 + 3.46\ ^5I_6 + 2.26\ ^5I_4$
12	$\Gamma_{2,3}$		1820	$95.21\ ^5I_5 + 2.89\ ^5I_4 + 1.49\ ^5I_6$
13	Γ_1		1857	$92.37\ ^5I_5 + 5.87\ ^5I_4 + 1.30\ ^5I_6$
14	Γ_1	$^5I_6$	3154	$99.26\ ^5I_6 + 0.27\ ^5I_7 + 0.17\ ^5I_4$
15	$\Gamma_{2,3}$	3186	3203	$98.69\ ^5I_6 + 0.46\ ^5I_5 + 0.42\ ^5I_7$
16	$\Gamma_{2,3}$		3309	$98.29\ ^5I_6 + 0.76\ ^5I_5 + 0.63\ ^5I_7$
17	Γ_1		3338	$96.14\ ^5I_6 + 3.12\ ^5I_7 + 0.36\ ^5I_8$
18	Γ_1		3359	$97.09\ ^5I_6 + 1.82\ ^5I_7 + 0.52\ ^5I_8$
19	$\Gamma_{2,3}$		3424	$96.11\ ^5I_6 + 1.78\ ^5I_5 + 1.59\ ^5I_7$
20	$\Gamma_{2,3}$		3429	$94.94\ ^5I_6 + 2.71\ ^5I_7 + 1.75\ ^5I_5$
21	Γ_1		3455	$97.79\ ^5I_6 + 1.50\ ^5I_5 + 0.62\ ^5I_7$
22	Γ_1		3462	$95.98\ ^5I_6 + 3.15\ ^5I_5 + 0.64\ ^5I_7$
23	Γ_1	$^5I_7$	4881	$99.36\ ^5I_7 + 0.23\ ^5I_8 + 0.11\ ^5I_5$
24	$\Gamma_{2,3}$	4876	4893	$98.68\ ^5I_7 + 0.68\ ^5I_8 + 0.28\ ^5I_6$
25	$\Gamma_{2,3}$		4936	$97.96\ ^5I_7 + 1.01\ ^5I_8 + 0.67\ ^5I_6$
26	Γ_1		4992	$98.20\ ^5I_7 + 0.97\ ^5I_6 + 0.70\ ^5I_8$
27	$\Gamma_{2,3}$		5039	$95.82\ ^5I_7 + 2.77\ ^5I_8 + 1.21\ ^5I_6$
28	Γ_1		5051	$97.04\ ^5I_7 + 2.45\ ^5I_6 + 0.32\ ^5I_5$
29	$\Gamma_{2,3}$		5103	$96.38\ ^5I_7 + 2.07\ ^5I_6 + 1.33\ ^5I_8$
30	$\Gamma_{2,3}$		5141	$93.94\ ^5I_7 + 4.28\ ^5I_8 + 1.24\ ^5I_6$
31	Γ_1		5217	$96.98\ ^5I_7 + 1.52\ ^5I_6 + 1.40\ ^5I_8$
32	Γ_1		5219	$97.16\ ^5I_7 + 1.53\ ^5I_6 + 1.25\ ^5I_8$
33	Γ_1	$^5I_8$	6529	$98.68\ ^5I_8 + 1.05\ ^5I_7 + 0.11\ ^5I_6$
34	$\Gamma_{2,3}$	6611	6548	$98.25\ ^5I_8 + 1.47\ ^5I_7 + 0.16\ ^5I_6$
35	$\Gamma_{2,3}$		6590	$96.63\ ^5I_8 + 3.26\ ^5I_7 + 0.03\ ^5F_4$
36	Γ_1		6599	$99.25\ ^5I_8 + 0.40\ ^5I_7 + 0.14\ ^5I_6$
37	$\Gamma_{2,3}$		6633	$98.63\ ^5I_8 + 1.04\ ^5I_7 + 0.16\ ^5I_6$
38	Γ_1		6795	$98.69\ ^5I_8 + 0.92\ ^5I_7 + 0.30\ ^5I_6$
39	$\Gamma_{2,3}$		6797	$97.28\ ^5I_8 + 2.50\ ^5I_7 + 0.11\ ^5I_6$
40	$\Gamma_{2,3}$		6986	$99.10\ ^5I_8 + 0.74\ ^5I_7 + 0.04\ ^5I_6$
41	Γ_1		7083	$99.04\ ^5I_8 + 0.60\ ^5I_7 + 0.28\ ^5I_6$
42	Γ_1		7104	$98.97\ ^5I_8 + 0.72\ ^5I_7 + 0.21\ ^5I_6$
43	$\Gamma_{2,3}$		7202	$98.74\ ^5I_8 + 1.16\ ^5I_7 + 0.03\ ^5F_5$
44	$\Gamma_{2,3}$	$^5F_1$	12460	$89.51\ ^5F_1 + 8.57\ ^5F_2 + 1.56\ ^5F_3$
45	Γ_1	12397	12671	$98.86\ ^5F_1 + 0.73\ ^5F_3 + 0.20\ ^5F_5$
46	$\Gamma_{2,3}$	$^5F_2$	12872	$93.52\ ^5F_2 + 3.34\ ^5F_1 + 2.11\ ^5F_3$
47	$\Gamma_{2,3}$	12811	12979	$92.47\ ^5F_2 + 5.57\ ^5F_1 + 1.01\ ^5F_3$
48	Γ_1		13215	$99.53\ ^5F_2 + 0.16\ ^5F_4 + 0.13\ ^5F_5$

Table 15 (cont'd). Predicted energy levels for Pm³⁺ in Ca₅(PO₄)₃F, C₃ site. Bₙₘ from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm⁻¹)	Free ion mixture (%)
49	Γ_1	$^5F_3$	13699	$93.55\ ^5F_3 + 5.73\ ^5F_4 + 0.44\ ^5F_5$
50	$\Gamma_{2,3}$	13651	13720	$96.27\ ^5F_3 + 2.74\ ^5F_2 + 0.39\ ^5F_5$
51	Γ_1		13780	$95.55\ ^5F_3 + 3.74\ ^5F_4 + 0.32\ ^5F_1$
52	$\Gamma_{2,3}$		13941	$96.75\ ^5F_3 + 1.06\ ^5F_1 + 1.03\ ^5F_4$
53	Γ_1		13956	$97.36\ ^5F_3 + 2.14\ ^5F_4 + 0.25\ ^5F_1$
54	$\Gamma_{2,3}$	$^5S_2$	14512	$99.51\ ^5S_2 + 0.34\ ^5F_4 + 0.04\ ^5I_8$
55	Γ_1	14337	14516	$99.81\ ^5S_2 + 0.06\ ^5F_4 + 0.05\ ^5I_8$
56	$\Gamma_{2,3}$		14520	$99.58\ ^5S_2 + 0.25\ ^5F_4 + 0.04\ ^5F_3$
57	$\Gamma_{2,3}$	$^5F_4$	14626	$96.50\ ^5F_4 + 2.63\ ^5F_5 + 0.53\ ^5F_3$
58	$\Gamma_{2,3}$	14561	14728	$97.89\ ^5F_4 + 0.71\ ^5F_2 + 0.51\ ^5F_5$
59	Γ_1		14770	$97.60\ ^5F_4 + 1.48\ ^5F_3 + 0.46\ ^5F_5$
60	$\Gamma_{2,3}$		14798	$97.56\ ^5F_4 + 0.92\ ^5F_5 + 0.71\ ^5F_3$
61	Γ_1		14809	$92.42\ ^5F_4 + 6.44\ ^5F_3 + 0.91\ ^5F_5$
62	Γ_1		14887	$95.80\ ^5F_4 + 3.83\ ^5F_3 + 0.11\ ^5F_5$
63	$\Gamma_{2,3}$	$^5F_5$	15771	$99.05\ ^5F_5 + 0.67\ ^3K_6 + 0.14\ ^5F_4$
64	$\Gamma_{2,3}$	15862	16006	$93.25\ ^3K_6 + 6.60\ ^5F_5 + 0.11\ ^5F_4$
65	Γ_1	$^3K_6$	16010	$57.52\ ^5F_5 + 41.71\ ^3K_6 + 0.50\ ^5F_4$
66	$\Gamma_{2,3}$	15874	16012	$94.66\ ^3K_6 + 5.20\ ^5F_5 + 0.11\ ^5F_4$
67	Γ_1		16022	$99.24\ ^3K_6 + 0.69\ ^5F_5 + 0.06\ ^5F_4$
68	Γ_1		16029	$61.17\ ^3K_6 + 38.51\ ^5F_5 + 0.17\ ^5F_4$
69	$\Gamma_{2,3}$		16041	$74.51\ ^5F_5 + 24.16\ ^3K_6 + 1.01\ ^5F_4$
70	Γ_1		16042	$97.85\ ^3K_6 + 2.02\ ^5F_5 + 0.08\ ^5F_4$
71	Γ_1		16042	$96.69\ ^3K_6 + 3.22\ ^5F_5 + 0.06\ ^5F_4$
72	$\Gamma_{2,3}$		16067	$94.58\ ^3K_6 + 5.33\ ^5F_5 + 0.05\ ^5F_4$
73	Γ_1		16096	$99.12\ ^3K_6 + 0.83\ ^5F_5 + 0.04\ ^5F_4$
74	$\Gamma_{2,3}$		16097	$82.70\ ^3K_6 + 16.87\ ^5F_5 + 0.36\ ^5F_4$
75	$\Gamma_{2,3}$		16154	$92.96\ ^5F_5 + 6.02\ ^3K_6 + 0.44\ ^5F_3$
76	$\Gamma_{2,3}$		16178	$94.01\ ^5F_5 + 3.74\ ^3K_6 + 1.95\ ^5F_4$
77	Γ_1		16200	$96.88\ ^5F_5 + 2.01\ ^3K_6 + 0.65\ ^5F_4$
78	Γ_1		16218	$97.33\ ^5F_5 + 1.88\ ^3K_6 + 0.36\ ^5F_4$

[a]Irreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.
[b]Aqueous centroids (cm⁻¹).

Table 16. Predicted energy levels for Sm³⁺ in Ca₅(PO₄)₃F, C₃ site. Bₙₘ from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm⁻¹)	Free ion mixture (%)
1	$\Gamma_{4,5}$	$^6H_{5/2}$	0	$95.35\ ^6H_{5/2} + 3.20\ ^6H_{7/2} + 1.00\ ^6H_{9/2}$
2	$^2\Gamma_6$	46	279	$88.50\ ^6H_{5/2} + 10.12\ ^6H_{7/2} + 0.83\ ^6H_{9/2}$
3	$\Gamma_{4,5}$		570	$97.98\ ^6H_{5/2} + 1.27\ ^6H_{7/2} + 0.43\ ^6H_{9/2}$
4	$^2\Gamma_6$	$^6H_{7/2}$	1227	$85.60\ ^6H_{7/2} + 10.69\ ^6H_{5/2} + 3.04\ ^6H_{9/2}$
5	$\Gamma_{4,5}$	1084	1234	$92.82\ ^6H_{7/2} + 3.42\ ^6H_{5/2} + 2.21\ ^6H_{9/2}$
6	$\Gamma_{4,5}$		1433	$94.34\ ^6H_{7/2} + 4.03\ ^6H_{9/2} + 0.84\ ^6H_{5/2}$
7	$\Gamma_{4,5}$		1630	$98.28\ ^6H_{7/2} + 0.88\ ^6H_{9/2} + 0.30\ ^6H_{5/2}$
8	$\Gamma_{4,5}$	$^6H_{9/2}$	2411	$89.65\ ^6H_{9/2} + 5.91\ ^6H_{7/2} + 2.86\ ^6H_{11/2}$
9	$^2\Gamma_6$	2299	2456	$93.27\ ^6H_{9/2} + 3.42\ ^6H_{7/2} + 2.57\ ^6H_{11/2}$
10	$\Gamma_{4,5}$		2562	$94.72\ ^6H_{9/2} + 1.55\ ^6H_{11/2} + 1.29\ ^6H_{7/2}$
11	$\Gamma_{4,5}$		2694	$96.20\ ^6H_{9/2} + 2.54\ ^6H_{11/2} + 0.48\ ^6H_{13/2}$
12	$^2\Gamma_6$		2858	$99.04\ ^6H_{9/2} + 0.34\ ^6H_{11/2} + 0.14\ ^6H_{7/2}$

20

Level	I. R.[a]	[(S,L)J][b]	Energy (cm^{-1})	Free ion mixture (%)
13	$\Gamma_{4,5}$	$^6H_{11/2}$	3729	90.82 $^6H_{11/2}$ + 4.56 $^6H_{9/2}$ + 2.80 $^6H_{13/2}$
14	$^2\Gamma_6$	3638	3763	92.92 $^6H_{11/2}$ + 2.91 $^6H_{13/2}$ + 2.37 $^6H_{9/2}$
15	$G_{4,5}$		3836	94.96 $^6H_{11/2}$ + 1.91 $^6H_{9/2}$ + 1.67 $^6H_{13/2}$
16	$\Gamma_{4,5}$		3932	94.60 $^6H_{11/2}$ + 2.69 $^6H_{13/2}$ + 1.39 $^6H_{9/2}$
17	$^2\Gamma_6$		4125	98.33 $^6H_{11/2}$ + 0.45 $^6F_{9/2}$ + 0.44 $^6H_{13/2}$
18	$\Gamma_{4,5}$		4203	99.25 $^6H_{11/2}$ + 0.20 $^6H_{13/2}$ + 0.14 $^6F_{11/2}$
19	$^2\Gamma_6$	$^6H_{13/2}$	5100	90.06 $^6H_{13/2}$ + 4.58 $^6H_{15/2}$ + 2.39 $^6H_{11/2}$
20	$\Gamma_{4,5}$	5060	5138	92.55 $^6H_{13/2}$ + 2.89 $^6H_{15/2}$ + 2.35 $^6H_{11/2}$
21	$\Gamma_{4,5}$		5165	92.52 $^6H_{13/2}$ + 2.65 $^6H_{11/2}$ + 2.63 $^6H_{15/2}$
22	$\Gamma_{4,5}$		5317	94.36 $^6H_{13/2}$ + 2.83 $^6H_{11/2}$ + 1.75 $^6H_{15/2}$
23	$^2\Gamma_6$		5500	98.24 $^6H_{13/2}$ + 0.51 $^6H_{11/2}$ + 0.50 $^6H_{15/2}$
24	$\Gamma_{4,5}$		5603	97.75 $^6H_{13/2}$ + 0.64 $^6F_{11/2}$ + 0.48 $^6F_{5/2}$
25	$\Gamma_{4,5}$		5610	98.74 $^6H_{13/2}$ + 0.27 $^6F_{11/2}$ + 0.25 $^6F_{5/2}$
26	$\Gamma_{4,5}$	$^6F_{1/2}$	6342	95.00 $^6H_{15/2}$ + 2.13 $^6H_{13/2}$ + 0.67 $^6H_{11/2}$
27	$^2\Gamma_6$	6422	6499	92.01 $^6H_{15/2}$ + 4.00 $^6H_{13/2}$ + 1.56 $^6F_{5/2}$
28	$\Gamma_{4,5}$	$^6H_{15/2}$	6696	91.22 $^6H_{15/2}$ + 2.97 $^6H_{13/2}$ + 2.22 $^6F_{5/2}$
29	$\Gamma_{4,5}$	6531	6798	92.24 $^6F_{1/2}$ + 2.35 $^6F_{3/2}$ + 2.15 $^6H_{15/2}$
30	$\Gamma_{4,5}$	$^6F_{3/2}$	6890	84.70 $^6H_{15/2}$ + 7.35 $^6F_{3/2}$ + 2.38 $^6F_{1/2}$
31	$^2\Gamma_6$	6666	6962	72.51 $^6H_{15/2}$ + 24.49 $^6F_{3/2}$ + 1.42 $^6F_{9/2}$
32	$\Gamma_{4,5}$		7032	52.60 $^6F_{3/2}$ + 40.71 $^6H_{15/2}$ + 3.33 $^6F_{5/2}$
33	$\Gamma_{4,5}$		7060	95.82 $^6H_{15/2}$ + 1.36 $^6F_{3/2}$ + 1.10 $^6F_{7/2}$
34	$^2\Gamma_6$		7069	77.32 $^6H_{15/2}$ + 17.85 $^6F_{3/2}$ + 2.92 $^6F_{5/2}$
35	$\Gamma_{4,5}$		7071	63.22 $^6H_{15/2}$ + 30.98 $^6F_{3/2}$ + 2.75 $^6F_{5/2}$
36	$^2\Gamma_6$		7107	53.93 $^6F_{3/2}$ + 43.44 $^6H_{15/2}$ + 1.07 $^6H_{13/2}$
37	$^2\Gamma_6$	$^6F_{5/2}$	7523	92.97 $^6F_{5/2}$ + 4.12 $^6H_{15/2}$ + 0.90 $^6H_{13/2}$
38	$\Gamma_{4,5}$	7158	7559	94.50 $^6F_{5/2}$ + 2.11 $^6F_{3/2}$ + 1.90 $^6H_{15/2}$
39	$\Gamma_{4,5}$		7611	92.07 $^6F_{5/2}$ + 5.65 $^6H_{15/2}$ + 1.04 $^6H_{13/2}$
40	$\Gamma_{4,5}$	$^6F_{7/2}$	8324	96.82 $^6F_{7/2}$ + 1.56 $^6H_{15/2}$ + 0.72 $^6H_{13/2}$
41	$\Gamma_{4,5}$	8006	8380	97.34 $^6F_{7/2}$ + 1.63 $^6H_{15/2}$ + 0.28 $^6H_{11/2}$
42	$^2\Gamma_6$		8424	97.13 $^6F_{7/2}$ + 1.11 $^6H_{15/2}$ + 0.42 $^6H_{11/2}$
43	$\Gamma_{4,5}$		8460	95.92 $^6F_{7/2}$ + 2.49 $^6H_{15/2}$ + 0.69 $^6H_{13/2}$
44	$\Gamma_{4,5}$	$^6F_{9/2}$	9490	98.30 $^6F_{9/2}$ + 0.54 $^6H_{13/2}$ + 0.54 $^6H_{15/2}$
45	$^2\Gamma_6$	9167	9508	97.28 $^6F_{9/2}$ + 1.62 $^6H_{15/2}$ + 0.30 $^6H_{11/2}$
46	$\Gamma_{4,5}$		9561	97.20 $^6F_{9/2}$ + 1.44 $^6H_{15/2}$ + 0.62 $^6H_{13/2}$
47	$^2\Gamma_6$		9565	97.87 $^6F_{9/2}$ + 0.96 $^6H_{15/2}$ + 0.36 $^6F_{11/2}$
48	$\Gamma_{4,5}$		9627	99.07 $^6F_{9/2}$ + 0.36 $^6F_{7/2}$ + 0.22 $^6H_{15/2}$
49	$\Gamma_{4,5}$	$^6F_{11/2}$	10804	97.23 $^6F_{11/2}$ + 1.59 $^6H_{15/2}$ + 0.89 $^6H_{13/2}$
50	$\Gamma_{4,5}$	10552	10915	99.43 $^6F_{11/2}$ + 0.19 $^6F_{9/2}$ + 0.19 $^6H_{15/2}$
51	$^2\Gamma_6$		10917	98.43 $^6F_{11/2}$ + 0.77 $^6H_{15/2}$ + 0.57 $^6F_{9/2}$
52	$^2\Gamma_6$		10969	98.97 $^6F_{11/2}$ + 0.60 $^6H_{15/2}$ + 0.22 $^6F_{9/2}$
53	$\Gamma_{4,5}$		10975	99.39 $^6F_{11/2}$ + 0.23 $^6H_{15/2}$ + 0.10 $^6F_{7/2}$
54	$\Gamma_{4,5}$		10997	99.20 $^6F_{11/2}$ + 0.44 $^6H_{15/2}$ + 0.16 $^6H_{13/2}$
55	$^2\Gamma_6$	$^4G_{5/2}$	17981	97.84 $^4G_{5/2}$ + 2.16 $^4F_{3/2}$
56	$\Gamma_{4,5}$	17935	18177	99.74 $^4G_{5/2}$ + 0.25 $^4F_{3/2}$
57	$\Gamma_{4,5}$		18596	99.86 $^4G_{5/2}$ + 0.14 $^4F_{3/2}$
58	$\Gamma_{4,5}$	$^4F_{3/2}$	19211	99.61 $^4F_{3/2}$ + 0.39 $^4G_{5/2}$
59	$^2\Gamma_6$	18899	19272	97.84 $^4F_{3/2}$ + 2.16 $^4G_{5/2}$

[a] Irreducible representations of C_3 double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.
[b] Aqueous centroids (cm^{-1}).

Table 17. Predicted energy levels for Eu^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^7F_0$ -31	0	$95.31\ ^7F_0 + 3.64\ ^7F_2 + 0.83\ ^7F_4$
2	$\Gamma_{2,3}$	$^7F_1$	295	$97.07\ ^7F_1 + 1.78\ ^7F_2 + 0.49\ ^7F_4$
3	Γ_1	350	574	$90.92\ ^7F_1 + 8.64\ ^7F_3 + 0.21\ ^7F_4$
4	$\Gamma_{2,3}$	$^7F_2$	936	$95.00\ ^7F_2 + 2.56\ ^7F_3 + 0.85\ ^7F_4$
5	$\Gamma_{2,3}$	1018	1020	$91.79\ ^7F_2 + 6.40\ ^7F_3 + 0.82\ ^7F_5$
6	Γ_1		1431	$85.91\ ^7F_2 + 8.49\ ^7F_3 + 2.97\ ^7F_0$
7	Γ_1	$^7F_3$	1826	$96.16\ ^7F_3 + 3.23\ ^7F_5 + 0.39\ ^7F_2$
8	Γ_1	1881	1870	$87.69\ ^7F_3 + 8.70\ ^7F_2 + 2.06\ ^7F_5$
9	$\Gamma_{2,3}$		1907	$87.84\ ^7F_3 + 10.17\ ^7F_4 + 0.70\ ^7F_5$
10	$\Gamma_{2,3}$		2081	$82.16\ ^7F_3 + 10.76\ ^7F_4 + 6.17\ ^7F_2$
11	Γ_1		2082	$90.22\ ^7F_3 + 8.68\ ^7F_1 + 0.48\ ^7F_5$
12	$\Gamma_{2,3}$	$^7F_4$	2714	$84.17\ ^7F_4 + 7.54\ ^7F_3 + 6.46\ ^7F_5$
13	Γ_1	2867	2925	$95.68\ ^7F_4 + 1.74\ ^7F_3 + 0.88\ ^7F_0$
14	$\Gamma_{2,3}$		3010	$90.20\ ^7F_4 + 3.71\ ^7F_5 + 3.29\ ^7F_3$
15	$\Gamma_{2,3}$		3039	$87.20\ ^7F_4 + 7.39\ ^7F_3 + 4.49\ ^7F_5$
16	Γ_1		3168	$96.36\ ^7F_4 + 2.07\ ^7F_6 + 0.80\ ^7F_5$
17	Γ_1		3229	$93.49\ ^7F_4 + 3.56\ ^7F_5 + 2.63\ ^7F_6$
18	Γ_1	$^7F_5$	3740	$96.85\ ^7F_5 + 1.98\ ^7F_3 + 0.87\ ^7F_4$
19	$\Gamma_{2,3}$	3928	3864	$93.66\ ^7F_5 + 3.44\ ^7F_4 + 1.58\ ^7F_6$
20	$\Gamma_{2,3}$		4016	$86.69\ ^7F_5 + 9.46\ ^7F_6 + 3.26\ ^7F_4$
21	$\Gamma_{2,3}$		4087	$90.38\ ^7F_5 + 7.34\ ^7F_6 + 1.74\ ^7F_4$
22	$\Gamma_{2,3}$		4172	$85.95\ ^7F_5 + 8.79\ ^7F_6 + 3.99\ ^7F_4$
23	Γ_1		4207	$95.68\ ^7F_5 + 2.04\ ^7F_6 + 1.60\ ^7F_3$
24	Γ_1		4319	$91.75\ ^7F_5 + 4.14\ ^7F_6 + 2.26\ ^7F_3$
25	Γ_1	$^7F_6$	4942	$98.12\ ^7F_6 + 1.49\ ^7F_4 + 0.17\ ^7F_2$
26	$\Gamma_{2,3}$	5029	4997	$96.68\ ^7F_6 + 2.30\ ^7F_5 + 0.53\ ^7F_3$
27	Γ_1		5029	$94.29\ ^7F_6 + 3.13\ ^7F_4 + 2.08\ ^7F_5$
28	$\Gamma_{2,3}$		5046	$95.82\ ^7F_6 + 2.26\ ^7F_5 + 1.42\ ^7F_4$
29	Γ_1		5161	$95.21\ ^7F_6 + 2.93\ ^7F_5 + 1.75\ ^7F_4$
30	$\Gamma_{2,3}$		5229	$88.13\ ^7F_6 + 10.14\ ^7F_5 + 1.50\ ^7F_4$
31	$\Gamma_{2,3}$		5456	$88.47\ ^7F_6 + 11.28\ ^7F_5 + 0.14\ ^7F_4$
32	Γ_1		5732	$99.68\ ^7F_6 + 0.13\ ^7F_5 + 0.08\ ^7F_4$
33	Γ_1		5732	$99.69\ ^7F_6 + 0.12\ ^7F_5 + 0.10\ ^7F_4$
34	Γ_1	$^5D_0$ 17286	17399	$99.85\ ^5D_0 + 0.10\ ^5L_6 + 0.05\ ^5D_2$
35	$\Gamma_{2,3}$	$^5D_1$	19109	$99.88\ ^5D_1 + 0.05\ ^5D_2 + 0.04\ ^5L_6$
36	Γ_1	19026	19220	$99.97\ ^5D_1 + 0.02\ ^5L_6$
37	$\Gamma_{2,3}$	$^5D_2$	21592	$99.79\ ^5D_2 + 0.16\ ^5D_3 + 0.04\ ^5L_6$
38	Γ_1	21499	21592	$99.85\ ^5D_2 + 0.09\ ^5L_6 + 0.05\ ^5D_0$
39	$\Gamma_{2,3}$		21660	$99.88\ ^5D_2 + 0.07\ ^5L_6 + 0.05\ ^5D_1$
40	Γ_1	$^5D_3$	24473	$99.92\ ^5D_3 + 0.07\ ^5L_6$
41	$\Gamma_{2,3}$	24390	24488	$99.81\ ^5D_3 + 0.11\ ^5D_2 + 0.07\ ^5L_6$
42	$\Gamma_{2,3}$		24500	$99.88\ ^5D_3 + 0.05\ ^5D_2 + 0.05\ ^5L_6$
43	Γ_1		24568	$99.89\ ^5D_3 + 0.10\ ^5L_6 + 0.01\ ^5D_2$
44	Γ_1		24582	$99.85\ ^5D_3 + 0.15\ ^5L_6$

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
				Table 17 (cont'd). Predicted energy levels for Eu^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_3$ site. B_{nm} from table 6.
45	G_1	$^5L_6$	25199	$99.76\ ^5L_6 + 0.17\ ^5D_3 + 0.07\ ^5D_2$
46	Γ_1	25375	25237	$99.95\ ^5L_6 + 0.04\ ^5D_3 + 0.01\ ^5D_1$
47	Γ_1		25252	$99.93\ ^5L_6 + 0.04\ ^5D_3 + 0.03\ ^5D_0$
48	$\Gamma_{2,3}$		25288	$99.89\ ^5L_6 + 0.06\ ^5D_3 + 0.04\ ^5D_2$
49	$\Gamma_{2,3}$		25463	$99.96\ ^5L_6 + 0.01\ ^5D_2 + 0.01\ ^5D_3$
50	$\Gamma_{2,3}$		25648	$99.93\ ^5L_6 + 0.05\ ^5D_3 + 0.02\ ^5D_2$
51	Γ_1		25690	$99.92\ ^5L_6 + 0.04\ ^5D_3 + 0.03\ ^5D_0$
52	Γ_1		25757	$99.91\ ^5L_6 + 0.04\ ^5D_0 + 0.04\ ^5D_3$
53	$\Gamma_{2,3}$		25791	$99.95\ ^5L_6 + 0.04\ ^5D_2 + 0.01\ ^5D_1$

[a]Irreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

[b]Aqueous centroids (cm^{-1}).

Table 18. Predicted energy levels for Gd^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_3$ site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	$\Gamma_{4,5}$	$^8S_{7/2}$	0	$100.00\ ^8S_{7/2}$
2	$^2\Gamma_6$	14	0.2	$100.00\ ^8S_{7/2}$
3	$\Gamma_{4,5}$		0.6	$100.00\ ^8S_{7/2}$
4	$\Gamma_{4,5}$		1.2	$100.00\ ^8S_{7/2}$
5	$\Gamma_{4,5}$	$^6P_{7/2}$	32096	$99.22\ ^6P_{7/2} + 0.13\ ^6P_{3/2} + 0.11\ ^6I_{13/2}$
6	$^2\Gamma_6$	32224	32116	$98.69\ ^6P_{7/2} + 0.53\ ^6P_{5/2} + 0.21\ ^6P_{3/2}$
7	$^2\Gamma_6$		32116	$98.69\ ^6P_{7/2} + 0.53\ ^6P_{5/2} + 0.21\ ^6P_{3/2}$
8	$\Gamma_{4,5}$		32185	$98.94\ ^6P_{7/2} + 0.42\ ^6P_{5/2} + 0.16\ ^6I_{17/2}$
9	$\Gamma_{4,5}$		32317	$99.20\ ^6P_{7/2} + 0.20\ ^6I_{15/2} + 0.15\ ^6I_{17/2}$
10	$\Gamma_{4,5}$	$^6P_{5/2}$	32663	$98.45\ ^6P_{5/2} + 0.44\ ^6I_{7/2} + 0.39\ ^6I_{17/2}$
11	$^2\Gamma_6$	32767	32673	$94.96\ ^6P_{5/2} + 3.45\ ^6P_{3/2} + 0.61\ ^6P_{7/2}$
12	$\Gamma_{4,5}$		32803	$98.87\ ^6P_{5/2} + 0.40\ ^6P_{7/2} + 0.27\ ^6I_{17/2}$
13	$^2\Gamma_6$	$^6P_{3/2}$	33235	$95.31\ ^6P_{3/2} + 3.58\ ^6P_{5/2} + 0.36\ ^6I_{13/2}$
14	$\Gamma_{4,5}$	33303	33294	$98.46\ ^6P_{3/2} + 0.33\ ^6P_{5/2} + 0.32\ ^6I_{15/2}$
15	$\Gamma_{4,5}$	$^6I_{7/2}$	35842	$99.59\ ^6I_{7/2} + 0.19\ ^6P_{5/2} + 0.08\ ^6I_{9/2}$
16	$^2\Gamma_6$	35879	35849	$99.18\ ^6I_{7/2} + 0.43\ ^6I_{9/2} + 0.27\ ^6P_{5/2}$
17	$\Gamma_{4,5}$		35882	$99.43\ ^6I_{7/2} + 0.25\ ^6P_{5/2} + 0.16\ ^6I_{9/2}$
18	$\Gamma_{4,5}$		35915	$99.69\ ^6I_{7/2} + 0.14\ ^6P_{5/2} + 0.06\ ^6I_{9/2}$
19	$\Gamma_{4,5}$	$^6I_{9/2}$	36184	$98.87\ ^6I_{9/2} + 0.56\ ^6I_{11/2} + 0.12\ ^6I_{7/2}$
20	$\Gamma_{4,5}$	36231	36201	$99.17\ ^6I_{9/2} + 0.25\ ^6I_{11/2} + 0.18\ ^6I_{17/2}$
21	$^2\Gamma_6$		36208	$98.63\ ^6I_{9/2} + 0.48\ ^6I_{11/2} + 0.40\ ^6I_{7/2}$
22	$\Gamma_{4,5}$		36235	$98.88\ ^6I_{9/2} + 0.29\ ^6I_{17/2} + 0.26\ ^6I_{11/2}$
23	$^2\Gamma_6$		36284	$99.42\ ^6I_{9/2} + 0.22\ ^6I_{13/2} + 0.09\ ^6I_{11/2}$
24	$\Gamma_{4,5}$	$^6I_{17/2}$	36441	$92.80\ ^6I_{17/2} + 4.96\ ^6I_{11/2} + 1.39\ ^6I_{15/2}$
25	$\Gamma_{4,5}$	36462	36442	$95.31\ ^6I_{17/2} + 2.13\ ^6I_{11/2} + 1.61\ ^6I_{15/2}$
26	$^2\Gamma_6$		36442	$96.81\ ^6I_{17/2} + 1.50\ ^6I_{15/2} + 1.32\ ^6I_{11/2}$
27	$^2\Gamma_6$		36446	$95.97\ ^6I_{17/2} + 2.09\ ^6I_{11/2} + 1.17\ ^6I_{15/2}$
28	$\Gamma_{4,5}$		36447	$91.83\ ^6I_{17/2} + 5.85\ ^6I_{11/2} + 1.61\ ^6I_{15/2}$
29	$\Gamma_{4,5}$		36452	$99.03\ ^6I_{17/2} + 0.62\ ^6I_{11/2} + 0.13\ ^6I_{13/2}$
30	$\Gamma_{4,5}$		36455	$89.72\ ^6I_{17/2} + 8.14\ ^6I_{11/2} + 0.78\ ^6I_{13/2}$
31	$^2\Gamma_6$		36456	$91.64\ ^6I_{17/2} + 6.87\ ^6I_{11/2} + 0.76\ ^6I_{13/2}$
32	$\Gamma_{4,5}$		36460	$91.98\ ^6I_{17/2} + 6.59\ ^6I_{11/2} + 0.48\ ^6I_{13/2}$

Table 18 (cont'd). Predicted energy levels for Gd^{3+} in Ca$_5$(PO$_4$)$_3$F, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
33	$\Gamma_{4,5}$	$^6I_{11/2}$	36479	81.65 $^6I_{11/2}$ +16.50 $^6I_{17/2}$ + 0.75 $^6I_{15/2}$
34	$\Gamma_{4,5}$	36526	36489	89.16 $^6I_{11/2}$ + 8.44 $^6I_{17/2}$ + 1.04 $^6I_{13/2}$
35	$^2\Gamma_6$		36499	90.62 $^6I_{11/2}$ + 7.37 $^6I_{17/2}$ + 0.79 $^6I_{15/2}$
36	$^2\Gamma_6$		36523	94.28 $^6I_{11/2}$ + 3.31 $^6I_{17/2}$ + 0.93 $^6I_{13/2}$
37	$\Gamma_{4,5}$		36533	94.74 $^6I_{11/2}$ + 4.16 $^6I_{17/2}$ + 0.44 $^6I_{15/2}$
38	$\Gamma_{4,5}$		36585	94.46 $^6I_{11/2}$ + 3.43 $^6I_{15/2}$ + 1.37 $^6I_{13/2}$
39	$\Gamma_{4,5}$	$^6I_{13/2}$	36657	81.93 $^6I_{13/2}$ +15.30 $^6I_{15/2}$ + 1.68 $^6I_{11/2}$
40	$^2\Gamma_6$	36711	36659	64.83 $^6I_{13/2}$ +31.53 $^6I_{15/2}$ + 1.73 $^6I_{17/2}$
41	$\Gamma_{4,5}$	$^6I_{15/2}$	36675	74.75 $^6I_{13/2}$ +21.51 $^6I_{15/2}$ + 2.34 $^6I_{11/2}$
42	$\Gamma_{4,5}$	36725	36692	57.14 $^6I_{15/2}$ +37.35 $^6I_{13/2}$ + 3.68 $^6I_{11/2}$
43	$^2\Gamma_6$		36694	59.74 $^6I_{15/2}$ +38.95 $^6I_{13/2}$ + 0.65 $^6I_{11/2}$
44	$\Gamma_{4,5}$		36698	67.53 $^6I_{15/2}$ +31.29 $^6I_{13/2}$ + 0.45 $^6I_{11/2}$
45	$\Gamma_{4,5}$		36702	75.67 $^6I_{15/2}$ +23.00 $^6I_{13/2}$ + 0.74 $^6I_{11/2}$
46	$^2\Gamma_6$		36707	68.98 $^6I_{13/2}$ +29.22 $^6I_{15/2}$ + 1.04 $^6I_{11/2}$
47	$\Gamma_{4,5}$		36715	77.76 $^6I_{13/2}$ +21.35 $^6I_{15/2}$ + 0.33 $^6I_{17/2}$
48	$\Gamma_{4,5}$		36725	77.69 $^6I_{15/2}$ +19.92 $^6I_{13/2}$ + 2.04 $^6I_{17/2}$
49	$^2\Gamma_6$		36731	77.10 $^6I_{15/2}$ +22.26 $^6I_{13/2}$ + 0.28 $^6I_{11/2}$
50	$\Gamma_{4,5}$		36734	49.57 $^6I_{13/2}$ +49.23 $^6I_{15/2}$ + 0.75 $^6I_{17/2}$
51	$\Gamma_{4,5}$		36742	83.78 $^6I_{15/2}$ +15.30 $^6I_{13/2}$ + 0.32 $^6I_{17/2}$
52	$^2\Gamma_6$		36782	97.13 $^6I_{15/2}$ + 1.82 $^6I_{17/2}$ + 0.79 $^6I_{13/2}$
53	$\Gamma_{4,5}$		36790	81.07 $^6I_{13/2}$ +18.70 $^6I_{15/2}$ + 0.06 $^6I_{11/2}$
54	$\Gamma_{4,5}$	$^6D_{9/2}$	39618	99.24 $^6D_{9/2}$ + 0.27 $^6D_{7/2}$ + 0.18 $^6D_{1/2}$
55	$^2\Gamma_6$	39779	39691	98.73 $^6D_{9/2}$ + 1.09 $^6D_{7/2}$ + 0.05 $^6P_{5/2}$
56	$\Gamma_{4,5}$		39809	99.06 $^6D_{9/2}$ + 0.74 $^6D_{7/2}$ + 0.06 $^6D_{5/2}$
57	$^2\Gamma_6$		39828	99.85 $^6D_{9/2}$ + 0.03 $^6I_{15/2}$ + 0.03 $^6D_{5/2}$
58	$\Gamma_{4,5}$		39882	99.59 $^6D_{9/2}$ + 0.16 $^6D_{7/2}$ + 0.12 $^6D_{1/2}$
59	$\Gamma_{4,5}$	$^6D_{1/2}$ 40621	40576	85.99 $^6D_{1/2}$ + 6.73 $^6D_{7/2}$ + 4.32 $^6D_{3/2}$
60	$\Gamma_{4,5}$	$^6D_{7/2}$ 40713	40680	90.88 $^6D_{7/2}$ + 4.65 $^6D_{3/2}$ + 3.69 $^6D_{5/2}$
61	$^2\Gamma_6$		40694	86.07 $^6D_{7/2}$ +12.11 $^6D_{3/2}$ + 1.07 $^6D_{9/2}$
62	$\Gamma_{4,5}$		40703	94.59 $^6D_{7/2}$ + 2.47 $^6D_{1/2}$ + 2.20 $^6D_{3/2}$
63	$\Gamma_{4,5}$		40727	88.07 $^6D_{7/2}$ + 5.04 $^6D_{1/2}$ + 3.64 $^6D_{5/2}$
64	$\Gamma_{4,5}$	$^6D_{3/2}$ 40851	40772	78.83 $^6D_{3/2}$ +12.14 $^6D_{7/2}$ + 8.12 $^6D_{5/2}$
65	$^2\Gamma_6$		40878	64.11 $^6D_{5/2}$ +30.79 $^6D_{3/2}$ + 4.94 $^6D_{7/2}$
66	$^2\Gamma_6$	$^6D_{5/2}$ 40978	40976	56.96 $^6D_{3/2}$ +35.11 $^6D_{5/2}$ + 7.71 $^6D_{7/2}$
67	$\Gamma_{4,5}$		41009	89.62 $^6D_{5/2}$ + 4.34 $^6D_{7/2}$ + 3.90 $^6D_{3/2}$
68	$\Gamma_{4,5}$		41056	91.53 $^6D_{5/2}$ + 3.64 $^6D_{1/2}$ + 3.07 $^6D_{3/2}$

[a]Irreducible representations of C_3 double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.
[b]Aqueous centroids (cm^{-1}).

Table 19. Predicted energy levels for Tb^{3+} in Ca$_5$(PO$_4$)$_3$F, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^7F_6$	0	99.86 $^7F_6$ + 0.04 $^7F_4$ + 0.04 $^7F_5$
2	Γ_1	74	0	99.86 $^7F_6$ + 0.04 $^7F_5$ + 0.03 $^7F_4$
3	$\Gamma_{2,3}$		335	95.82 $^7F_6$ + 4.06 $^7F_5$ + 0.08 $^7F_4$
4	$\Gamma_{2,3}$		560	96.69 $^7F_6$ + 2.73 $^7F_5$ + 0.46 $^7F_4$
5	Γ_1		606	98.64 $^7F_6$ + 0.69 $^7F_5$ + 0.61 $^7F_4$
6	$\Gamma_{2,3}$		706	98.73 $^7F_6$ + 0.55 $^7F_5$ + 0.48 $^7F_4$
7	Γ_1		721	98.43 $^7F_6$ + 0.97 $^7F_4$ + 0.37 $^7F_5$
8	$\Gamma_{2,3}$		746	99.05 $^7F_6$ + 0.49 $^7F_5$ + 0.23 $^7F_3$
9	Γ_1		786	99.29 $^7F_6$ + 0.49 $^7F_4$ + 0.10 $^7F_2$
10	Γ_1	$^7F_5$	2353	95.27 $^7F_5$ + 2.02 $^7F_4$ + 1.86 $^7F_3$
11	$\Gamma_{2,3}$	2112	2450	92.50 $^7F_5$ + 3.78 $^7F_4$ + 3.03 $^7F_6$
12	Γ_1		2456	97.52 $^7F_5$ + 1.27 $^7F_3$ + 0.64 $^7F_4$
13	$\Gamma_{2,3}$		2532	96.27 $^7F_5$ + 2.73 $^7F_6$ + 0.58 $^7F_4$
14	$\Gamma_{2,3}$		2594	94.64 $^7F_5$ + 2.56 $^7F_4$ + 2.02 $^7F_6$
15	$\Gamma_{2,3}$		2786	96.00 $^7F_5$ + 2.60 $^7F_4$ + 0.47 $^7F_2$
16	Γ_1		2906	97.87 $^7F_5$ + 1.45 $^7F_3$ + 0.48 $^7F_4$
17	Γ_1	$^7F_4$	3622	95.83 $^7F_4$ + 2.80 $^7F_5$ + 0.89 $^7F_6$
18	Γ_1	3370	3684	97.66 $^7F_4$ + 0.78 $^7F_5$ + 0.72 $^7F_6$
19	$\Gamma_{2,3}$		3804	86.71 $^7F_4$ + 8.84 $^7F_3$ + 3.65 $^7F_5$
20	$\Gamma_{2,3}$		3829	93.62 $^7F_4$ + 2.22 $^7F_5$ + 1.76 $^7F_3$
21	Γ_1		3916	95.92 $^7F_4$ + 1.32 $^7F_2$ + 1.24 $^7F_3$
22	$\Gamma_{2,3}$		4097	86.88 $^7F_4$ + 6.56 $^7F_3$ + 4.84 $^7F_5$
23	Γ_1	$^7F_3$	4712	85.50 $^7F_3$ + 13.75 $^7F_1$ + 0.44 $^7F_5$
24	$\Gamma_{2,3}$	4344	4746	80.96 $^7F_3$ + 10.35 $^7F_4$ + 8.08 $^7F_2$
25	$\Gamma_{2,3}$		4919	88.39 $^7F_3$ + 9.95 $^7F_4$ + 0.70 $^7F_2$
26	Γ_1		4941	79.78 $^7F_3$ + 17.11 $^7F_2$ + 1.43 $^7F_5$
27	Γ_1		4998	96.82 $^7F_3$ + 2.37 $^7F_5$ + 0.44 $^7F_2$
28	Γ_1	$^7F_2$	5242	74.42 $^7F_2$ + 17.40 $^7F_3$ + 4.65 $^7F_0$
29	$\Gamma_{2,3}$	5028	5646	89.62 $^7F_2$ + 8.31 $^7F_3$ + 0.96 $^7F_1$
30	$\Gamma_{2,3}$		5716	93.76 $^7F_2$ + 3.32 $^7F_3$ + 1.42 $^7F_1$
31	Γ_1	$^7F_1$	5903	85.84 $^7F_1$ + 13.76 $^7F_3$ + 0.24 $^7F_4$
32	$\Gamma_{2,3}$	5481	6156	95.78 $^7F_1$ + 3.13 $^7F_2$ + 0.50 $^7F_4$
33	Γ_1	$^7F_0$ 5703	6307	92.51 $^7F_0$ + 6.39 $^7F_2$ + 0.94 $^7F_4$
34	Γ_1	$^5D_4$	20931	99.75 $^5D_4$ + 0.15 $^5G_6$ + 0.05 $^5L_{10}$
35	Γ_1	20542	20942	99.78 $^5D_4$ + 0.12 $^5G_6$ + 0.04 $^5L_{10}$
36	$\Gamma_{2,3}$		20970	99.86 $^5D_4$ + 0.07 $^5G_6$ + 0.04 $^5L_{10}$
37	$\Gamma_{2,3}$		21026	99.76 $^5D_4$ + 0.07 $^5G_6$ + 0.06 $^5L_{10}$
38	$\Gamma_{2,3}$		21106	99.81 $^5D_4$ + 0.06 $^5L_{10}$ + 0.05 $^5G_5$
39	Γ_1		21127	99.83 $^5D_4$ + 0.06 $^5L_{10}$ + 0.05 $^5G_4$
40	Γ_1	$^5D_3$	26470	92.51 $^5G_6$ + 3.80 $^5D_3$ + 2.39 $^5L_{10}$
41	Γ_1	26336	26482	95.42 $^5G_6$ + 2.51 $^5L_{10}$ + 1.00 $^5L_9$
42	$\Gamma_{2,3}$	$^5G_6$	26732	58.62 $^5D_3$ + 38.18 $^5G_6$ + 1.26 $^5L_{10}$
43	Γ_1	26425	26759	83.54 $^5D_3$ + 14.38 $^5G_6$ + 1.26 $^5G_5$
44	$\Gamma_{2,3}$		26765	65.09 $^5D_3$ + 32.74 $^5G_6$ + 1.06 $^5L_{10}$
45	Γ_1		26767	87.56 $^5D_3$ + 10.38 $^5G_6$ + 1.31 $^5G_5$
46	Γ_1		26785	84.32 $^5D_3$ + 14.02 $^5G_6$ + 0.92 $^5G_5$
47	$\Gamma_{2,3}$		26836	58.38 $^5G_6$ + 36.29 $^5D_3$ + 3.11 $^5L_{10}$

Table 19 (cont'd). Predicted energy levels for Tb^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
48	$\Gamma_{2,3}$		26867	$86.82\ ^5G_6 + 9.24\ ^5D_3 + 2.28\ ^5L_{10}$
49	Γ_1		26922	$90.36\ ^5G_6 + 6.16\ ^5D_3 + 2.89\ ^5L_{10}$
50	Γ_1		26996	$73.49\ ^5G_6 + 24.25\ ^5D_3 + 1.74\ ^5L_{10}$
51	$\Gamma_{2,3}$		27050	$80.13\ ^5G_6 + 16.40\ ^5D_3 + 2.54\ ^5L_{10}$
52	$\Gamma_{2,3}$		27106	$82.43\ ^5G_6 + 12.12\ ^5D_3 + 4.43\ ^5L_{10}$
53	Γ_1		27130	$87.25\ ^5G_6 + 7.18\ ^5L_{10} + 4.40\ ^5D_3$
54	$\Gamma_{2,3}$	$^5L_{10}$	27332	$95.93\ ^5L_{10} + 2.19\ ^5G_6 + 0.96\ ^5G_5$
55	Γ_1	27146	27344	$97.56\ ^5L_{10} + 1.94\ ^5G_6 + 0.25\ ^5G_5$
56	Γ_1		27363	$91.29\ ^5L_{10} + 8.23\ ^5G_6 + 0.14\ ^5G_4$
57	$\Gamma_{2,3}$		27389	$93.87\ ^5L_{10} + 4.99\ ^5G_6 + 0.67\ ^5L_9$
58	$\Gamma_{2,3}$		27508	$96.10\ ^5L_{10} + 1.55\ ^5G_6 + 1.50\ ^5L_9$
59	$\Gamma_{2,3}$		27564	$95.70\ ^5L_{10} + 2.70\ ^5G_6 + 1.24\ ^5L_9$
60	Γ_1		27645	$96.71\ ^5L_{10} + 1.44\ ^5L_9 + 0.99\ ^5G_6$
61	Γ_1		27689	$96.23\ ^5L_{10} + 2.04\ ^5G_6 + 1.43\ ^5L_9$
62	Γ_1		27697	$95.90\ ^5L_{10} + 1.77\ ^5G_6 + 1.49\ ^5L_9$
63	Γ_1		27716	$96.63\ ^5L_{10} + 1.75\ ^5G_5 + 1.16\ ^5L_9$
64	$\Gamma_{2,3}$		27814	$95.58\ ^5L_{10} + 2.33\ ^5G_5 + 1.14\ ^5G_6$
65	$\Gamma_{2,3}$		27909	$92.71\ ^5L_{10} + 5.15\ ^5G_5 + 1.53\ ^5G_6$
66	Γ_1		27948	$93.04\ ^5L_{10} + 4.70\ ^5G_5 + 1.89\ ^5G_6$
67	$\Gamma_{2,3}$		27953	$97.68\ ^5L_{10} + 1.86\ ^5G_5 + 0.37\ ^5G_6$
68	$\Gamma_{2,3}$	$^5G_5$	28104	$93.33\ ^5G_5 + 1.86\ ^5G_6 + 1.56\ ^5G_4$
69	$\Gamma_{2,3}$	277795	28179	$79.93\ ^5G_5 + 11.76\ ^5G_4 + 5.33\ ^5L_{10}$
70	Γ_1		28297	$93.17\ ^5G_5 + 2.74\ ^5L_{10} + 2.51\ ^5D_2$
71	Γ_1		28320	$91.88\ ^5G_5 + 3.94\ ^5L_{10} + 2.53\ ^5D_2$
72	$\Gamma_{2,3}$		28343	$89.56\ ^5G_5 + 6.07\ ^5D_2 + 3.07\ ^5L_{10}$
73	$\Gamma_{2,3}$		28403	$88.48\ ^5G_5 + 6.87\ ^5D_2 + 2.57\ ^5G_4$
74	Γ_1		28480	$91.53\ ^5G_5 + 5.36\ ^5G_4 + 1.71\ ^5L_{10}$
75	Γ_1	$^5D_2$	28567	$88.95\ ^5D_2 + 4.31\ ^5G_4 + 4.08\ ^5G_5$
76	$\Gamma_{2,3}$	28150	28620	$75.81\ ^5D_2 + 19.61\ ^5G_4 + 3.24\ ^5G_5$
77	$\Gamma_{2,3}$		28698	$64.04\ ^5D_2 + 24.07\ ^5G_4 + 9.27\ ^5G_5$
78	Γ_1	$^5G_4$	28715	$70.96\ ^5G_4 + 27.42\ ^5L_9 + 0.44\ ^5G_6$
79	Γ_1	28307	28727	$57.80\ ^5G_4 + 35.61\ ^5L_9 + 3.95\ ^5G_5$
80	$\Gamma_{2,3}$	$^5L_9$	28757	$45.16\ ^5G_4 + 42.06\ ^5L_9 + 9.91\ ^5G_5$
81	$\Gamma_{2,3}$	28503	28814	$65.89\ ^5L_9 + 20.94\ ^5G_4 + 9.12\ ^5D_2$
82	Γ_1		28815	$66.18\ ^5L_9 + 32.86\ ^5G_4 + 0.37\ ^5L_{10}$
83	Γ_1		28827	$66.85\ ^5L_9 + 30.56\ ^5G_4 + 1.46\ ^5G_5$
84	$\Gamma_{2,3}$		28843	$44.73\ ^5G_4 + 41.36\ ^5L_9 + 11.72\ ^5D_2$
85	$\Gamma_{2,3}$		28892	$50.74\ ^5L_9 + 39.37\ ^5G_4 + 4.53\ ^5G_5$
86	$\Gamma_{2,3}$		28918	$52.28\ ^5G_4 + 33.92\ ^5L_9 + 12.71\ ^5D_2$
87	Γ_1		28919	$69.33\ ^5G_4 + 27.70\ ^5L_9 + 2.26\ ^5D_2$
88	$\Gamma_{2,3}$		28963	$70.76\ ^5L_9 + 24.04\ ^5G_4 + 3.55\ ^5D_2$
89	$\Gamma_{2,3}$		29018	$94.78\ ^5L_9 + 2.69\ ^5G_4 + 1.64\ ^5L_{10}$
90	Γ_1		29042	$91.35\ ^5L_9 + 7.12\ ^5G_4 + 0.69\ ^5L_{10}$
91	Γ_1		29104	$82.25\ ^5L_9 + 16.14\ ^5G_4 + 1.17\ ^5L_{10}$
92	$\Gamma_{2,3}$		29186	$92.17\ ^5L_9 + 6.39\ ^5G_4 + 0.72\ ^5L_{10}$
93	Γ_1		29199	$97.54\ ^5L_9 + 1.46\ ^5L_{10} + 0.64\ ^5G_4$
94	Γ_1		29201	$96.80\ ^5L_9 + 1.43\ ^5L_{10} + 1.36\ ^5G_4$
95	$\Gamma_{2,3}$		29253	$95.96\ ^5L_9 + 2.89\ ^5G_4 + 0.40\ ^5G_6$
96	Γ_1		29273	$97.90\ ^5L_9 + 1.47\ ^5G_4 + 0.36\ ^5G_6$

[a]Irreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.

[b]Aqueous centroids (cm^{-1}).

	Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
Table 20. Predicted energy levels for Dy^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.	1	$\Gamma_{4,5}$	$^6H_{15/2}$	0	$99.68\ ^6H_{15/2} + 0.23\ ^6F_{11/2} + 0.04\ ^6H_{11/2}$
	2	$^2\Gamma_6$	40	1	$99.84\ ^6H_{15/2} + 0.12\ ^6F_{11/2} + 0.01\ ^6F_{9/2}$
	3	$\Gamma_{4,5}$		32	$99.93\ ^6H_{15/2} + 0.02\ ^6F_{7/2} + 0.01\ ^6H_{13/2}$
	4	$^2\Gamma_6$		77	$99.65\ ^6H_{15/2} + 0.12\ ^6H_{13/2} + 0.11\ ^6F_{11/2}$
	5	$\Gamma_{4,5}$		199	$99.23\ ^6H_{15/2} + 0.53\ ^6H_{13/2} + 0.13\ ^6F_{11/2}$
	6	$\Gamma_{4,5}$		412	$99.14\ ^6H_{15/2} + 0.69\ ^6H_{13/2} + 0.08\ ^6F_{11/2}$
	7	$^2\Gamma_6$		600	$99.24\ ^6H_{15/2} + 0.56\ ^6H_{13/2} + 0.08\ ^6H_{11/2}$
	8	$\Gamma_{4,5}$		721	$99.60\ ^6H_{15/2} + 0.14\ ^6H_{11/2} + 0.13\ ^6H_{13/2}$
	9	$\Gamma_{4,5}$	$^6H_{13/2}$	3443	$99.01\ ^6H_{13/2} + 0.75\ ^6F_{11/2} + 0.13\ ^6H_{11/2}$
	10	$\Gamma_{4,5}$	3506	3481	$99.80\ ^6H_{13/2} + 0.12\ ^6F_{11/2} + 0.02\ ^6F_{9/2}$
	11	$^2\Gamma_6$		3622	$99.57\ ^6H_{13/2} + 0.17\ ^6H_{11/2} + 0.10\ ^6H_{15/2}$
	12	$\Gamma_{4,5}$		3769	$98.40\ ^6H_{13/2} + 0.77\ ^6H_{11/2} + 0.53\ ^6H_{15/2}$
	13	$\Gamma_{4,5}$		3858	$97.42\ ^6H_{13/2} + 1.32\ ^6H_{11/2} + 0.73\ ^6H_{15/2}$
	14	$^2\Gamma_6$		3919	$97.86\ ^6H_{13/2} + 0.99\ ^6H_{11/2} + 0.60\ ^6H_{15/2}$
	15	$\Gamma_{4,5}$		3950	$99.11\ ^6H_{13/2} + 0.31\ ^6H_{11/2} + 0.26\ 6H_{9/2}$
	16	$\Gamma_{4,5}$	$^6H_{11/2}$	5753	$99.16\ ^6H_{11/2} + 0.55\ ^6F_{11/2} + 0.14\ ^6H_{13/2}$
	17	$^2\Gamma_6$	5833	5895	$97.73\ ^6H_{11/2} + 0.98\ ^6F_{11/2} + 0.92\ ^6F_{9/2}$
	18	$\Gamma_{4,5}$		6082	$97.22\ ^6H_{11/2} + 1.03\ ^6H_{9/2} + 0.68\ ^6H_{13/2}$
	19	$\Gamma_{4,5}$		6160	$97.41\ ^6H_{11/2} + 0.82\ ^6H_{13/2} + 0.80\ ^6H_{9/2}$
	20	$^2\Gamma_6$		6177	$96.78\ ^6H_{11/2} + 1.25\ ^6H_{9/2} + 1.08\ ^6H_{13/2}$
	21	$\Gamma_{4,5}$		6191	$97.19\ ^6H_{11/2} + 1.19\ ^6H_{9/2} + 0.76\ ^6H_{13/2}$
	22	$^2\Gamma_6$	$^6H_{9/2}$	7584	$83.00\ ^6H_{9/2} + 15.56\ ^6F_{11/2} + 1.12\ ^6F_{9/2}$
	23	$\Gamma_{4,5}$	7692	7737	$66.52\ ^6H_{9/2} + 31.27\ ^6F_{11/2} + 1.39\ ^6H_{11/2}$
	24	$\Gamma_{4,5}$	$^6F_{11/2}$	7826	$54.57\ ^6H_{9/2} + 42.45\ ^6F_{11/2} + 1.45\ ^6H_{7/2}$
	25	$^2\Gamma_6$	7730	7903	$92.74\ ^6F_{11/2} + 6.00\ ^6H_{9/2} + 0.62\ ^6H_{11/2}$
	26	$\Gamma_{4,5}$	$^6F_{9/2}$	7913	$74.26\ ^6F_{11/2} + 24.56\ ^6H_{9/2} + 0.33\ ^6H_{11/2}$
	27	$\Gamma_{4,5}$	9087	7949	$87.90\ ^6F_{11/2} + 10.89\ ^6H_{9/2} + 0.54\ ^6H_{7/2}$
	28	$\Gamma_{4,5}$	$^6H_{7/2}$	8001	$56.34\ ^6H_{9/2} + 40.69\ ^6F_{11/2} + 0.91\ ^6H_{7/2}$
	29	$^2\Gamma_6$	9115	8025	$52.03\ ^6H_{9/2} + 44.31\ ^6F_{11/2} + 1.41\ ^6F_{9/2}$
	30	$\Gamma_{4,5}$		8049	$61.74\ ^6H_{9/2} + 35.05\ ^6F_{11/2} + 1.76\ ^6H_{7/2}$
	31	$^2\Gamma_6$		8100	$52.62\ ^6H_{9/2} + 44.60\ ^6F_{11/2} + 0.86\ ^6H_{11/2}$
	32	$\Gamma_{4,5}$		8346	$83.00\ ^6F_{11/2} + 11.97\ ^6H_{9/2} + 2.40\ ^6H_{7/2}$
	33	$\Gamma_{4,5}$		8991	$68.08\ ^6H_{7/2} + 30.28\ ^6F_{9/2} + 0.54\ ^6F_{11/2}$
	34	$\Gamma_{4,5}$		9263	$52.21\ ^6F_{9/2} + 43.52\ ^6H_{7/2} + 3.10\ ^6H_{9/2}$
	35	$\Gamma_{4,5}$		9274	$61.34\ ^6F_{9/2} + 34.78\ ^6H_{7/2} + 1.49\ ^6H_{9/2}$
	36	$^2\Gamma_6$		9287	$81.55\ ^6F_{9/2} + 14.90\ ^6H_{7/2} + 2.42\ ^6H_{5/2}$
	37	$^2\Gamma_6$		9359	$66.03\ ^6F_{9/2} + 30.28\ ^6H_{7/2} + 1.59\ ^6H_{5/2}$
	38	$\Gamma_{4,5}$		9368	$55.13\ ^6H_{7/2} + 42.33\ ^6F_{9/2} + 0.83\ ^6H_{5/2}$
	39	$\Gamma_{4,5}$		9456	$66.60\ ^6F_{9/2} + 30.07\ ^6H_{7/2} + 1.06\ ^6H_{9/2}$
	40	$\Gamma_{4,5}$		9503	$53.60\ ^6H_{7/2} + 40.23\ ^6F_{9/2} + 3.35\ ^6H_{5/2}$
	41	$^2\Gamma_6$		9600	$46.21\ ^6F_{9/2} + 42.51\ ^6H_{7/2} + 6.90\ ^6H_{5/2}$
	42	$\Gamma_{4,5}$	$^6H_{5/2}$	10174	$93.38\ ^6H_{5/2} + 2.36\ ^6F_{7/2} + 2.22\ ^6F_{9/2}$
	43	$^2\Gamma_6$	10168	10423	$85.46\ ^6H_{5/2} + 9.64\ ^6H_{7/2} + 2.05\ ^6F_{7/2}$
	44	$\Gamma_{4,5}$		10687	$91.00\ ^6H_{5/2} + 5.34\ ^6F_{7/2} + 2.12\ ^6H_{7/2}$
	45	$\Gamma_{4,5}$	$^6F_{7/2}$	11239	$98.16\ ^6F_{7/2} + 0.66\ ^6H_{7/2} + 0.52\ ^6H_{5/2}$
	46	$^2\Gamma_6$	11025	11281	$96.24\ ^6F_{7/2} + 1.97\ ^6H_{5/2} + 0.84\ ^6F_{5/2}$
	47	$\Gamma_{4,5}$		11349	$95.39\ ^6F_{7/2} + 2.44\ ^6H_{5/2} + 0.67\ ^6H_{7/2}$
	48	$\Gamma_{4,5}$		11407	$93.45\ ^6F_{7/2} + 3.65\ ^6H_{5/2} + 1.01\ ^6F_{5/2}$

27

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
49	$\Gamma_{4,5}$	$^6F_{5/2}$	12655	$97.69\ ^6F_{5/2} + 1.20\ ^6F_{3/2} + 0.44\ ^6H_{5/2}$
50	$\Gamma_{4,5}$	12432	12705	$97.29\ ^6F_{5/2} + 0.70\ ^6F_{3/2} + 0.69\ ^6H_{7/2}$
51	$^2\Gamma_6$		12767	$96.67\ ^6F_{5/2} + 1.62\ ^6F_{3/2} + 0.52\ ^6F_{7/2}$
52	$^2\Gamma_6$	$^6F_{3/2}$	13489	$97.28\ ^6F_{3/2} + 1.34\ ^6F_{5/2} + 0.85\ ^6H_{5/2}$
53	$\Gamma_{4,5}$	13212	13498	$93.92\ ^6F_{3/2} + 3.81\ ^6F_{1/2} + 1.54\ ^6F_{5/2}$
54	$\Gamma_{4,5}$	$^6F_{1/2}$ 13760	14060	$95.11\ ^6F_{1/2} + 3.33\ ^6F_{3/2} + 0.50\ ^6H_{5/2}$
55	$\Gamma_{4,5}$	$^4F_{9/2}$	21143	$97.63\ ^4F_{9/2} + 1.81\ ^4I_{15/2} + 0.55\ ^4G_{11/2}$
56	$\Gamma_{4,5}$	21144	21303	$97.79\ ^4F_{9/2} + 1.88\ ^4I_{15/2} + 0.33\ ^4G_{11/2}$
57	$^2\Gamma_6$		21314	$97.61\ ^4F_{9/2} + 1.22\ ^4G_{11/2} + 1.16\ ^4I_{15/2}$
58	$\Gamma_{4,5}$		21407	$99.10\ ^4F_{9/2} + 0.84\ ^4I_{15/2} + 0.05\ ^4G_{11/2}$
59	$^2\Gamma_6$		21537	$92.80\ ^4F_{9/2} + 5.00\ ^4I_{15/2} + 2.20\ ^4G_{11/2}$
60	$\Gamma_{4,5}$	$^4I_{15/2}$	22213	$99.57\ ^4I_{15/2} + 0.30\ ^4G_{11/2} + 0.13\ ^4F_{9/2}$
61	$\Gamma_{4,5}$	22293	22282	$98.82\ ^4I_{15/2} + 1.06\ ^4G_{11/2} + 0.12\ ^4F_{9/2}$
62	$^2\Gamma_6$		22413	$94.96\ ^4I_{15/2} + 4.90\ ^4F_{9/2} + 0.14\ ^4G_{11/2}$
63	$^2\Gamma_6$		22576	$99.36\ ^4I_{15/2} + 0.48\ ^4G_{11/2} + 0.16\ ^4F_{9/2}$
64	$\Gamma_{4,5}$		22609	$94.40\ ^4I_{15/2} + 3.40\ ^4G_{11/2} + 2.20\ ^4F_{9/2}$
65	$\Gamma_{4,5}$		22696	$95.48\ ^4I_{15/2} + 3.59\ ^4G_{11/2} + 0.93\ ^4F_{9/2}$
66	$^2\Gamma_6$		22710	$94.88\ ^4I_{15/2} + 4.14\ ^4G_{11/2} + 0.97\ ^4F_{9/2}$
67	$\Gamma_{4,5}$		22730	$96.66\ ^4I_{15/2} + 2.12\ ^4G_{11/2} + 1.22\ ^4F_{9/2}$
68	$\Gamma_{4,5}$	$^4G_{11/2}$	23278	$97.69\ ^4G_{11/2} + 2.24\ ^4I_{15/2} + 0.07\ ^4F_{9/2}$
69	$^2\Gamma_6$	23321	23594	$95.95\ ^4G_{11/2} + 3.21\ ^4F_{9/2} + 0.84\ ^4I_{15/2}$
70	$\Gamma_{4,5}$		23625	$98.74\ ^4G_{11/2} + 0.75\ ^4I_{15/2} + 0.50\ ^4F_{9/2}$
71	$\Gamma_{4,5}$		23660	$99.05\ ^4G_{11/2} + 0.76\ ^4I_{15/2} + 0.18\ ^4F_{9/2}$
72	$^2\Gamma_6$		23706	$95.86\ ^4G_{11/2} + 3.80\ ^4I_{15/2} + 0.34\ ^4F_{9/2}$
73	$\Gamma_{4,5}$		23759	$93.10\ ^4G_{11/2} + 6.79\ ^4I_{15/2} + 0.11\ ^4F_{9/2}$

[a]Irreducible representations of C_3 double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.
[b]Aqueous centroids (cm^{-1}).

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	$\Gamma_{2,3}$	$^5I_8$	0	$99.89\ ^5I_8 + 0.09\ ^5I_7 + 0.01\ ^5F_5$
2	Γ_1	80	73	$99.91\ ^5I_8 + 0.05\ ^5I_7 + 0.02\ ^5I_6$
3	Γ_1		86	$99.91\ ^5I_8 + 0.05\ ^5I_7 + 0.03\ ^5I_6$
4	$\Gamma_{2,3}$		157	$99.93\ ^5I_8 + 0.05\ ^5I_7$
5	Γ_1		327	$99.87\ ^5I_8 + 0.06\ ^5I_7 + 0.03\ ^5G_6$
6	$\Gamma_{2,3}$		330	$99.79\ ^5I_8 + 0.16\ ^5I_7 + 0.02\ ^5G_6$
7	$\Gamma_{2,3}$		420	$99.86\ ^5I_8 + 0.07\ ^5I_7 + 0.03\ ^5G_6$
8	Γ_1		444	$99.90\ ^5I_8 + 0.04\ ^5G_6 + 0.02\ ^5I_7$
9	$\Gamma_{2,3}$		460	$99.81\ ^5I_8 + 0.16\ ^5I_7 + 0.01\ ^5G_6$
10	$\Gamma_{2,3}$		480	$99.88\ ^5I_8 + 0.07\ ^5I_7 + 0.02\ ^5G_6$
11	Γ_1		496	$99.89\ ^5I_8 + 0.05\ ^5I_7 + 0.02\ ^5G_6$
12	Γ_1	$^5I_7$	5200	$99.74\ ^5I_7 + 0.16\ ^5I_6 + 0.08\ ^5I_8$
13	Γ_1	5116	5201	$99.71\ ^5I_7 + 0.17\ ^5I_6 + 0.09\ ^5I_8$
14	$\Gamma_{2,3}$		5238	$99.53\ ^5I_7 + 0.24\ ^5I_8 + 0.14\ ^5I_6$
15	$\Gamma_{2,3}$		5278	$99.67\ ^5I_7 + 0.24\ ^5I_8 + 0.04\ ^5I_6$
16	$\Gamma_{2,3}$		5324	$99.55\ ^5I_7 + 0.36\ ^5I_6 + 0.04\ ^5I_8$
17	Γ_1		5362	$99.56\ ^5I_7 + 0.30\ ^5I_6 + 0.06\ ^5I_5$

	Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
Table 21 (cont'd). Predicted energy levels for Ho^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_3$ site. B_{nm} from table 6.	18	Γ_1		5389	$99.75\ ^5I_7 + 0.15\ ^5I_6 + 0.04\ ^5I_8$
	19	$\Gamma_{2,3}$		5435	$99.78\ ^5I_7 + 0.07\ ^5I_6 + 0.05\ ^5I_5$
	20	$\Gamma_{2,3}$		5466	$99.84\ ^5I_7 + 0.04\ ^5I_8 + 0.03\ ^5F_5$
	21	Γ_1		5475	$99.86\ ^5I_7 + 0.05\ ^5F_5 + 0.02\ ^5I_8$
	22	Γ_1	$^5I_6$	8757	$99.30\ ^5I_6 + 0.44\ ^5I_5 + 0.20\ ^5I_7$
	23	$\Gamma_{2,3}$	8614	8758	$99.49\ ^5I_6 + 0.26\ ^5I_5 + 0.16\ ^5I_7$
	24	Γ_1		8759	$99.45\ ^5I_6 + 0.32\ ^5I_5 + 0.16\ ^5I_7$
	25	$\Gamma_{2,3}$		8761	$99.11\ ^5I_6 + 0.37\ ^5I_7 + 0.37\ ^5I_5$
	26	Γ_1		8809	$99.48\ ^5I_6 + 0.25\ ^5I_7 + 0.12\ ^5I_5$
	27	Γ_1		8818	$99.40\ ^5I_6 + 0.30\ ^5I_5 + 0.15\ ^5I_7$
	28	$\Gamma_{2,3}$		8890	$99.51\ ^5I_6 + 0.29\ ^5I_5 + 0.06\ ^5F_5$
	29	$\Gamma_{2,3}$		8972	$99.72\ ^5I_6 + 0.08\ ^5I_5 + 0.07\ ^5I_4$
	30	Γ_1		9005	$99.85\ ^5I_6 + 0.04\ ^5I_4 + 0.03\ ^5F_4$
	31	$\Gamma_{2,3}$	$^5I_5$	11308	$98.88\ ^5I_5 + 0.63\ ^5I_4 + 0.38\ ^5I_6$
	32	$\Gamma_{2,3}$	11164	11322	$99.30\ ^5I_5 + 0.37\ ^5I_6 + 0.22\ ^5I_4$
	33	Γ_1		11329	$97.72\ ^5I_5 + 1.72\ ^5I_4 + 0.38\ ^5I_6$
	34	Γ_1		11345	$98.35\ ^5I_5 + 0.79\ ^5I_6 + 0.75\ ^5I_4$
	35	$\Gamma_{2,3}$		11425	$99.54\ ^5I_5 + 0.18\ ^5I_4 + 0.17\ ^5I_6$
	36	$\Gamma_{2,3}$		11490	$99.18\ ^5I_5 + 0.61\ ^5I_4 + 0.07\ ^5I_6$
	37	Γ_1		11535	$99.78\ ^5I_5 + 0.08\ ^5F_5 + 0.03\ ^5F_1$
	38	Γ_1	$^5I_4$	13218	$99.23\ ^5I_4 + 0.58\ ^5I_5 + 0.11\ ^5I_6$
	39	Γ_1	13219	13329	$98.14\ ^5I_4 + 1.75\ ^5I_5 + 0.06\ ^5I_6$
	40	$\Gamma_{2,3}$		13363	$99.14\ ^5I_4 + 0.64\ ^5I_5 + 0.13\ ^5I_6$
	41	$\Gamma_{2,3}$		13520	$98.98\ ^5I_4 + 0.82\ ^5I_5 + 0.05\ ^5I_6$
	42	Γ_1		13568	$99.59\ ^5I_4 + 0.15\ ^5I_5 + 0.11\ ^5S_2$
	43	$\Gamma_{2,3}$		13635	$99.65\ ^5I_4 + 0.18\ ^5I_5 + 0.05\ ^5F_3$
	44	Γ_1	$^5F_5$	15602	$99.38\ ^5F_5 + 0.34\ ^5G_6 + 0.13\ ^5F_4$
	45	Γ_1	15519	15620	$99.31\ ^5F_5 + 0.35\ ^5G_6 + 0.18\ ^5F_4$
	46	$\Gamma_{2,3}$		15653	$99.32\ ^5F_5 + 0.29\ ^5F_4 + 0.23\ ^5G_6$
	47	$\Gamma_{2,3}$		15670	$99.39\ ^5F_5 + 0.25\ ^5G_6 + 0.15\ ^5F_4$
	48	$\Gamma_{2,3}$		15771	$99.52\ ^5F_5 + 0.15\ ^5F_4 + 0.11\ ^5G_6$
	49	Γ_1		15800	$99.68\ ^5F_5 + 0.08\ ^5I_5 + 0.07\ ^5F_4$
	50	$\Gamma_{2,3}$		15950	$99.87\ ^5F_5 + 0.05\ ^3G_5 + 0.03\ ^5G_6$
	51	Γ_1	$^5S_2$	18558	$93.92\ ^5S_2 + 5.72\ ^5F_4 + 0.17\ ^5G_6$
	52	$\Gamma_{2,3}$	18353	18571	$95.68\ ^5S_2 + 3.99\ ^5F_4 + 0.20\ ^5G_6$
	53	$\Gamma_{2,3}$		18588	$97.36\ ^5S_2 + 2.27\ ^5F_4 + 0.18\ ^5G_6$
	54	Γ_1	$^5F_4$	18682	$93.62\ ^5F_4 + 5.37\ ^5S_2 + 0.56\ ^5G_6$
	55	$\Gamma_{2,3}$	18612	18747	$95.14\ ^5F_4 + 3.97\ ^5S_2 + 0.49\ ^5G_6$
	56	Γ_1		18849	$98.84\ ^5F_4 + 0.54\ ^5F_3 + 0.18\ ^5G_6$
	57	$\Gamma_{2,3}$		18857	$97.07\ ^5F_4 + 2.13\ ^5S_2 + 0.24\ ^5F_2$
	58	Γ_1		18884	$98.46\ ^5F_4 + 0.91\ ^5F_3 + 0.17\ ^5F_5$
	59	$\Gamma_{2,3}$		18968	$98.93\ ^5F_4 + 0.53\ ^5F_5 + 0.18\ ^5S_2$
	60	Γ_1	$^5F_3$	20759	$98.84\ ^5F_3 + 0.62\ ^3G_5 + 0.24\ ^5F_4$
	61	$\Gamma_{2,3}$	20672	20805	$97.81\ ^5F_3 + 1.15\ ^5F_2 + 0.47\ ^3G_5$
	62	Γ_1		20949	$98.02\ ^5F_3 + 0.95\ ^5G_6 + 0.72\ ^5F_4$
	63	$\Gamma_{2,3}$		20976	$93.11\ ^5F_3 + 6.06\ ^5F_2 + 0.37\ ^5G_6$
	64	Γ_1		20990	$98.08\ ^5F_3 + 0.85\ ^5F_4 + 0.77\ ^5G_6$

Table 21 (cont'd). Predicted energy levels for Ho^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
65	Γ_1	$^5F_2$	21252	$98.50\,^5F_2 + 0.98\,^5G_6 + 0.31\,^3K_8$
66	$\Gamma_{2,3}$	21130	21371	$94.83\,^5F_2 + 2.36\,^5F_3 + 1.22\,^3K_8$
67	$\Gamma_{2,3}$		21430	$90.77\,^5F_2 + 4.35\,^5F_3 + 3.23\,^3K_8$
68	Γ_1	$^3K_8$	21467	$99.31\,^3K_8 + 0.49\,^5G_6 + 0.18\,^5F_2$
69	$\Gamma_{2,3}$	21307	21471	$98.34\,^3K_8 + 1.04\,^5F_2 + 0.50\,^5G_6$
70	$\Gamma_{2,3}$		21481	$98.26\,^3K_8 + 1.47\,^5F_2 + 0.22\,^5F_3$
71	Γ_1		21483	$99.48\,^3K_8 + 0.36\,^5G_6 + 0.11\,^5F_2$
72	$\Gamma_{2,3}$		21491	$98.32\,^3K_8 + 1.25\,^5F_2 + 0.35\,^5G_6$
73	Γ_1		21518	$98.54\,^3K_8 + 1.39\,^5G_6 + 0.03\,^5F_2$
74	$\Gamma_{2,3}$		21524	$99.32\,^3K_8 + 0.32\,^5G_6 + 0.26\,^5F_2$
75	$\Gamma_{2,3}$		21597	$99.64\,^3K_8 + 0.18\,^5G_6 + 0.15\,^5F_2$
76	Γ_1		21616	$98.18\,^3K_8 + 1.69\,^5G_6 + 0.11\,^5F_3$
77	Γ_1		21622	$98.65\,^3K_8 + 1.27\,^5G_6 + 0.07\,^5F_3$
78	$\Gamma_{2,3}$		21654	$99.88\,^3K_8 + 0.10\,^5G_6 + 0.01\,^5F_2$
79	Γ_1	$^5G_6$	22181	$97.77\,^5G_6 + 0.67\,^5F_2 + 0.63\,^3K_8$
80	Γ_1	22094	22191	$96.85\,^5G_6 + 1.90\,^3K_8 + 0.89\,^5F_1$
81	Γ_1	$^5F_1$	22209	$96.93\,^5G_6 + 2.04\,^3K_8 + 0.37\,^5F_3$
82	$\Gamma_{2,3}$	22375	22229	$97.30\,^5G_6 + 0.58\,^5F_2 + 0.58\,^3G_5$
83	$\Gamma_{2,3}$		22320	$97.43\,^5G_6 + 0.89\,^3G_5 + 0.62\,^5F_1$
84	$\Gamma_{2,3}$		22420	$97.05\,^5G_6 + 1.19\,^5F_1 + 0.85\,^3G_5$
85	Γ_1		22467	$66.37\,^5G_6 + 32.81\,^5F_1 + 0.28\,^3K_8$
86	Γ_1		22513	$73.74\,^5G_6 + 25.05\,^5F_1 + 0.35\,^3K_8$
87	$\Gamma_{2,3}$		22516	$94.51\,^5G_6 + 3.16\,^5F_1 + 0.98\,^3G_5$
88	Γ_1		22554	$58.01\,^5G_6 + 40.80\,^5F_1 + 0.60\,^5F_3$
89	$\Gamma_{2,3}$		22703	$93.02\,^5F_1 + 5.42\,^5G_6 + 0.73\,^5F_2$
90	Γ_1	$^3G_5$	24043	$99.23\,^3G_5 + 0.67\,^5F_3 + 0.04\,^5F_5$
91	$\Gamma_{2,3}$	23887	24065	$98.77\,^3G_5 + 0.41\,^5G_6 + 0.34\,^5F_3$
92	$\Gamma_{2,3}$		24096	$98.84\,^3G_5 + 0.63\,^5G_6 + 0.20\,^5F_2$
93	Γ_1		24158	$99.73\,^3G_5 + 0.12\,^5G_6 + 0.10\,^5F_4$
94	Γ_1		24175	$99.62\,^3G_5 + 0.19\,^5G_6 + 0.05\,^5F_4$
95	$\Gamma_{2,3}$		24219	$98.50\,^3G_5 + 1.19\,^5G_6 + 0.11\,^5F_2$
96	$\Gamma_{2,3}$		24265	$98.76\,^3G_5 + 0.98\,^5G_6 + 0.10\,^5F_4$

[a] Irreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.
[b] Aqueous centroids (cm^{-1}).

Table 22. Predicted energy levels for Tm^{3+} in $Ca_5(PO_4)_3F$, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^3H_6$	0	$99.76\,^3H_6 + 0.20\,^3F_4 + 0.02\,^3H_4$
2	$\Gamma_{2,3}$	202	56	$99.82\,^3H_6 + 0.12\,^3F_4 + 0.03\,^3F_3$
3	$\Gamma_{2,3}$		186	$99.79\,^3H_6 + 0.14\,^3F_4 + 0.03\,^3H_5$
4	Γ_1		329	$99.56\,^3H_6 + 0.35\,^3F_4 + 0.06\,^3H_5$
5	Γ_1		418	$99.60\,^3H_6 + 0.28\,^3F_4 + 0.09\,^3H_5$
6	$\Gamma_{2,3}$		657	$99.60\,^3H_6 + 0.32\,^3F_4 + 0.06\,^3H_5$
7	Γ_1		659	$99.90\,^3H_6 + 0.08\,^3F_4 + 0.01\,^3H_4$
8	Γ_1		661	$99.88\,^3H_6 + 0.10\,^3F_4 + 0.01\,^3H_4$
9	$\Gamma_{2,3}$		896	$99.95\,^3H_6 + 0.03\,^3H_5 + 0.01\,^3F_3$

Table 22 (cont'd). Predicted energy levels for Tm^{3+} in Ca$_5$(PO$_4$)$_3$F, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	[(S,L)J][b]	Energy (cm^{-1})	Free ion mixture (%)
10	$\Gamma_{2,3}$	$^3F_4$	5834	99.46 $^3F_4$ + 0.25 $^3H_6$ + 0.21 $^3H_5$
11	Γ_1	5812	5843	99.66 $^3F_4$ + 0.13 $^3H_4$ + 0.11 $^3H_5$
12	$\Gamma_{2,3}$		6068	99.03 $^3F_4$ + 0.71 $^3H_5$ + 0.17 $^3H_6$
13	Γ_1		6171	99.10 $^3F_4$ + 0.57 $^3H_6$ + 0.31 $^3H_5$
14	Γ_1		6211	98.50 $^3F_4$ + 1.00 $^3H_5$ + 0.47 $^3H_6$
15	$\Gamma_{2,3}$		6226	99.35 $^3F_4$ + 0.38 $^3H_5$ + 0.17 $^3H_6$
16	Γ_1	$^3H_5$	8263	99.72 $^3H_5$ + 0.18 $^3F_4$ + 0.07 $^3F_3$
17	$\Gamma_{2,3}$	8390	8312	98.90 $^3H_5$ + 0.72 $^3F_4$ + 0.14 $^3F_2$
18	$\Gamma_{2,3}$		8460	99.38 $^3H_5$ + 0.23 $^3F_3$ + 0.20 $^3H_4$
19	Γ_1		8697	99.17 $^3H_5$ + 0.35 $^3F_3$ + 0.33 $^3F_4$
20	Γ_1		8748	98.55 $^3H_5$ + 0.93 $^3F_4$ + 0.37 $^3F_3$
21	$\Gamma_{2,3}$		8893	99.68 $^3H_5$ + 0.22 $^3F_4$ + 0.03 $^3F_2$
22	$\Gamma_{2,3}$		8969	99.49 $^3H_5$ + 0.27 $^3F_4$ + 0.17 $^3H_4$
23	$\Gamma_{2,3}$	$^3H_4$	12715	98.26 $^3H_4$ + 0.97 $^3F_2$ + 0.52 $^3F_3$
24	Γ_1	12720	12744	98.44 $^3H_4$ + 1.34 $^3F_3$ + 0.12 $^3F_4$
25	$\Gamma_{2,3}$		12875	98.66 $^3H_4$ + 0.95 $^3F_2$ + 0.20 $^3H_5$
26	$\Gamma_{2,3}$		13102	99.11 $^3H_4$ + 0.46 $^3F_3$ + 0.18 $^3H_5$
27	Γ_1		13160	97.74 $^3H_4$ + 2.02 $^3F_3$ + 0.12 $^3H_5$
28	Γ_1		13240	97.15 $^3H_4$ + 2.63 $^3F_3$ + 0.08 $^3H_5$
29	Γ_1	$^3F_3$	14675	97.39 $^3F_3$ + 2.19 $^3H_4$ + 0.31 $^3H_5$
30	Γ_1		14742	95.56 $^3F_3$ + 3.80 $^3H_4$ + 0.30 $^3F_2$
31	$\Gamma_{2,3}$		14763	96.88 $^3F_3$ + 2.65 $^3F_2$ + 0.26 $^3H_5$
32	Γ_1		14801	99.79 $^3F_3$ + 0.10 $^3H_5$ + 0.07 $^3H_4$
33	$\Gamma_{2,3}$		14845	94.36 $^3F_3$ + 4.84 $^3F_2$ + 0.61 $^3H_4$
34	$\Gamma_{2,3}$	$^3F_2$	15277	95.30 $^3F_2$ + 3.11 $^3F_3$ + 1.38 $^3H_4$
35	$\Gamma_{2,3}$	15116	15445	94.71 $^3F_2$ + 4.03 $^3F_3$ + 1.02 $^3H_4$
36	Γ_1		15597	99.33 $^3F_2$ + 0.34 $^3F_3$ + 0.12 $^3H_4$
37	Γ_1	$^1G_4$	21188	99.86 $^1G_4$ + 0.05 $^3P_2$ + 0.03 $^3F_3$
38	$\Gamma_{2,3}$	21374	21322	99.78 $^1G_4$ + 0.05 $^3F_3$ + 0.05 $^1I_6$
39	$\Gamma_{2,3}$		21697	99.84 $^1G_4$ + 0.09 $^1I_6$ + 0.03 $^3H_4$
40	$\Gamma_{2,3}$		21802	99.72 $^1G_4$ + 0.17 $^1D_2$ + 0.03 $^1I_6$
41	Γ_1		21816	99.88 $^1G_4$ + 0.04 $^3F_3$ + 0.04 $^1I_6$
42	Γ_1		21904	99.90 $^1G_4$ + 0.05 $^1I_6$ + 0.03 $^3H_5$
43	$\Gamma_{2,3}$	$^1D_2$	28098	99.69 $^1D_2$ + 0.17 $^1G_4$ + 0.10 $^1I_6$
44	$\Gamma_{2,3}$	28032	28387	99.60 $^1D_2$ + 0.21 $^3P_1$ + 0.06 $^1I_6$
45	Γ_1		28451	99.77 $^1D_2$ + 0.07 $^3F_2$ + 0.04 $^3P_0$
46	Γ_1	$^1I_6$	34674	99.96 $^1I_6$ + 0.02 $^1G_4$ + 0.02 $^3P_2$
47	$\Gamma_{2,3}$	34886	34716	99.63 $^1I_6$ + 0.26 $^3P_2$ + 0.07 $^1D_2$
48	$\Gamma_{2,3}$	$^3P_0$	34793	99.68 $^1I_6$ + 0.22 $^3P_2$ + 0.06 $^1D_2$
49	Γ_1	35637	34824	99.95 $^1I_6$ + 0.04 $^1G_4$ + 0.01 $^3P_0$
50	Γ_1	$^3P_1$	34946	99.71 $^1I_6$ + 0.21 $^3P_0$ + 0.03 $^1G_4$
51	$\Gamma_{2,3}$	36297	35030	99.79 $^1I_6$ + 0.10 $^1G_4$ + 0.06 $^3P_2$
52	$\Gamma_{2,3}$		35356	99.91 $^1I_6$ + 0.06 $^3P_2$ + 0.01 $^1D_2$
53	Γ_1		35880	98.18 $^3P_0$ + 0.90 $^3P_2$ + 0.81 $^1I_6$
54	Γ_1		36289	58.43 $^3P_1$ + 41.56 $^1I_6$ + 0.01 $^3F_3$
55	Γ_1		36295	99.17 $^1I_6$ + 0.64 $^3P_0$ + 0.08 $^3P_1$
56	Γ_1		36298	58.51 $^1I_6$ + 41.48 $^3P_1$
57	$\Gamma_{2,3}$		36677	97.84 $^3P_1$ + 1.87 $^3P_2$ + 0.20 $^1D_2$

Table 22 (cont'd). Predicted energy levels for Tm^{3+} in Ca$_5$(PO$_4$)$_3$F, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
58	$\Gamma_{2,3}$	$^3P_2$	38196	99.47 $^3P_2$ + 0.37 $^1I_6$ + 0.12 $^3P_1$
59	$\Gamma_{2,3}$	38193	38525	97.96 $^3P_2$ + 1.74 $^3P_1$ + 0.22 $^1I_6$
60	Γ_1		38960	98.89 $^3P_2$ + 0.84 $^3P_0$ + 0.17 $^1I_6$
61	Γ_1	$^1S_0$ 79592	79855	99.97 $^1S_0$ + 0.01 $^3P_2$ + 0.01 $^1G_4$

[a]Irreducible representations of C_3 single group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$.
[b]Aqueous centroid (cm^{-1}).

Table 23. Predicted energy levels for Yb^{3+} in Ca$_5$(PO$_4$)$_3$F, C_3 site. B_{nm} from table 6.

Level	I. R.[a]	$[(S,L)J]$[b]	Energy (cm^{-1})	Free ion mixture (%)
1	$^2\Gamma_6$	$^2F_{7/2}$	0	99.97 $^2F_{7/2}$ + 0.03 $^2F_{5/2}$
2	$\Gamma_{4,5}$	250	52	99.92 $^2F_{7/2}$ + 0.08 $^2F_{5/2}$
3	$\Gamma_{4,5}$		318	99.96 $^2F_{7/2}$ + 0.04 $^2F_{5/2}$
4	$\Gamma_{4,5}$		891	99.98 $^2F_{7/2}$ + 0.02 $^2F_{5/2}$
5	$^2\Gamma_6$	$^2F_{5/2}$	10231	99.97 $^2F_{5/2}$ + 0.03 $^2F_{7/2}$
6	$\Gamma_{4,5}$	10450	10359	99.94 $^2F_{5/2}$ + 0.06 $^2F_{7/2}$
7	$\Gamma_{4,5}$		10988	99.92 $^2F_{5/2}$ + 0.08 $^2F_{7/2}$

[a]Irreducible representations of C_3 double group, $\Gamma_{4,5} = \Gamma_4 + \Gamma_5$.
[b]Aqueous centroids (cm^{-1}).

Table 24. Predicted energy levels for Ce^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	$[(S,L)J]$[a]	Energy (cm^{-1})	Free ion mixture (%)
1	$^2F_{5/2}$	0	98.03 $^2F_{5/2}$ + 1.97 $^2F_{7/2}$
2	250	561	93.72 $^2F_{5/2}$ + 6.28 $^2F_{7/2}$
3		1263	90.08 $^2F_{5/2}$ + 9.92 $^2F_{7/2}$
4	$^2F_{7/2}$	2330	93.56 $^2F_{7/2}$ + 6.44 $^2F_{5/2}$
5	2550	2819	92.32 $^2F_{7/2}$ + 7.68 $^2F_{5/2}$
6		3455	98.45 $^2F_{7/2}$ + 1.55 $^2F_{5/2}$
7		3859	97.50 $^2F_{7/2}$ + 2.50 $^2F_{5/2}$

[a]Aqueous centroids (cm^{-1}).

Table 25. Predicted energy levels for Pr^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]$[a]	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^3H_4$	0	98.23 $^3H_4$ + 1.09 $^3H_5$ + 0.29 $^3F_2$
2	Γ_1	245	61	97.36 $^3H_4$ + 2.10 $^3H_5$ + 0.23 $^3F_3$
3	Γ_2		509	95.53 $^3H_4$ + 3.07 $^3H_5$ + 1.07 $^3F_2$
4	Γ_1		636	97.19 $^3H_4$ + 1.51 $^3H_5$ + 0.82 $^3F_2$
5	Γ_2		655	97.81 $^3H_4$ + 1.58 $^3H_5$ + 0.41 $^3F_2$
6	Γ_2		766	97.00 $^3H_4$ + 2.32 $^3H_5$ + 0.50 $^3F_2$
7	Γ_1		1072	97.42 $^3H_4$ + 1.29 $^3F_2$ + 0.93 $^3H_5$
8	Γ_1		1151	98.36 $^3H_4$ + 0.58 $^3F_3$ + 0.53 $^3H_5$
9	Γ_2		1240	97.59 $^3H_4$ + 1.50 $^3H_5$ + 0.77 $^3F_3$

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
10	Γ_2	$^3H_5$	2164	$95.69\,^3H_5 + 2.09\,^3H_4 + 1.03\,^3H_6$
11	Γ_2	2323	2205	$94.50\,^3H_5 + 3.27\,^3H_4 + 1.51\,^3H_6$
12	Γ_1		2587	$94.67\,^3H_5 + 2.26\,^3H_4 + 1.12\,^3F_3$
13	Γ_2		2643	$95.94\,^3H_5 + 1.78\,^3H_6 + 1.37\,^3F_3$
14	Γ_1		2654	$94.93\,^3H_5 + 2.65\,^3H_6 + 1.33\,^3H_4$
15	Γ_1		2702	$94.74\,^3H_5 + 2.91\,^3H_6 + 1.06\,^3F_2$
16	Γ_2		2970	$95.42\,^3H_5 + 1.55\,^3F_2 + 1.28\,^3H_4$
17	Γ_2		3051	$97.46\,^3H_5 + 0.90\,^3F_3 + 0.72\,^3H_4$
18	Γ_1		3085	$94.18\,^3H_5 + 1.50\,^3H_4 + 1.49\,^3H_6$
19	Γ_1		3196	$95.79\,^3H_5 + 1.38\,^3H_6 + 1.05\,^3F_2$
20	Γ_2		3200	$96.33\,^3H_5 + 1.27\,^3F_2 + 0.92\,^3F_4$
21	Γ_1	$^3H_6$	4214	$95.37\,^3H_6 + 2.23\,^3H_5 + 1.13\,^3F_4$
22	Γ_1	4496	4226	$94.14\,^3H_6 + 3.41\,^3H_5 + 1.27\,^3F_4$
23	Γ_2		4558	$94.47\,^3H_6 + 2.28\,^3H_5 + 1.77\,^3F_4$
24	Γ_1		4669	$93.45\,^3H_6 + 3.38\,^3F_4 + 1.25\,^3H_5$
25	Γ_2		4748	$95.19\,^3H_6 + 1.79\,^3H_5 + 1.26\,^3F_2$
26	Γ_2		4875	$96.45\,^3H_6 + 1.50\,^3F_4 + 0.89\,^3F_3$
27	Γ_1		5066	$92.29\,^3H_6 + 3.95\,^3F_2 + 1.77\,^3F_3$
28	Γ_1		5116	$92.89\,^3H_6 + 3.52\,^3F_3 + 1.99\,^3F_4$
29	Γ_2		5192	$82.42\,^3H_6 + 15.26\,^3F_2 + 0.97\,^3F_4$
30	Γ_2		5280	$88.59\,^3H_6 + 3.86\,^3F_2 + 3.73\,^3F_4$
31	Γ_1		5327	$84.53\,^3H_6 + 10.92\,^3F_2 + 1.82\,^3F_4$
32	Γ_1		5351	$87.51\,^3H_6 + 4.50\,^3F_2 + 4.15\,^3F_4$
33	Γ_2		5374	$92.93\,^3H_6 + 3.14\,^3F_3 + 2.72\,^3F_4$
34	Γ_1	$^3F_2$	5648	$80.91\,^3F_2 + 15.29\,^3H_6 + 2.11\,^3H_5$
35	Γ_2	5149	5738	$81.02\,^3F_2 + 15.94\,^3H_6 + 1.22\,^3H_5$
36	Γ_2		5774	$89.46\,^3F_2 + 4.86\,^3H_6 + 2.91\,^3H_5$
37	Γ_1		5873	$93.89\,^3F_2 + 2.37\,^3H_6 + 1.64\,^3H_5$
38	Γ_1		5907	$91.77\,^3F_2 + 4.80\,^3H_6 + 1.59\,^3H_5$
39	Γ_2	$^3F_3$	7012	$93.14\,^3F_3 + 5.32\,^3F_4 + 0.76\,^3H_6$
40	Γ_1	6540	7014	$82.56\,^3F_3 + 11.98\,^3F_4 + 3.68\,^3H_6$
41	Γ_1		7070	$80.00\,^3F_3 + 13.53\,^3F_4 + 4.69\,^3H_6$
42	Γ_2		7128	$87.40\,^3F_3 + 5.92\,^3F_4 + 3.69\,^3H_6$
43	Γ_1		7160	$58.99\,^3F_3 + 34.45\,^3F_4 + 3.06\,^3H_6$
44	Γ_2		7177	$67.64\,^3F_3 + 27.02\,^3F_4 + 3.56\,^3H_6$
45	Γ_2		7267	$83.86\,^3F_3 + 11.55\,^3F_4 + 2.77\,^3H_6$
46	Γ_1	$^3F_4$	7297	$88.69\,^3F_4 + 7.68\,^3F_3 + 1.41\,^1G_4$
47	Γ_1	6973	7390	$64.44\,^3F_4 + 32.78\,^3F_3 + 1.53\,^1G_4$
48	Γ_2		7403	$62.76\,^3F_4 + 32.72\,^3F_3 + 2.77\,^3H_6$
49	Γ_1		7509	$74.57\,^3F_4 + 15.91\,^3F_3 + 8.01\,^3H_6$
50	Γ_2		7538	$83.05\,^3F_4 + 12.97\,^3F_3 + 3.11\,^3H_6$
51	Γ_2		7643	$97.09\,^3F_4 + 1.20\,^3H_6 + 0.80\,^3H_5$
52	Γ_1		7771	$94.26\,^3F_4 + 2.94\,^3F_3 + 1.38\,^3H_6$
53	Γ_2		7865	$90.96\,^3F_4 + 4.96\,^3F_3 + 3.25\,^3H_6$
54	Γ_1		7870	$94.45\,^3F_4 + 2.57\,^3H_6 + 1.90\,^3F_3$
55	Γ_2	$^1G_4$	9967	$97.40\,^1G_4 + 1.07\,^3F_4 + 0.90\,^3H_6$
56	Γ_1	9885	9982	$96.96\,^1G_4 + 2.08\,^3F_4 + 0.35\,^3H_6$
57	Γ_1		10015	$97.92\,^1G_4 + 1.24\,^3F_4 + 0.40\,^3H_6$
58	Γ_1		10135	$98.08\,^1G_4 + 0.91\,^3H_6 + 0.40\,^3F_4$

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
59	Γ_2		10417	$99.42\ ^1G_4 + 0.14\ ^3H_6 + 0.11\ ^3F_4$
60	Γ_2		10535	$99.27\ ^1G_4 + 0.26\ ^1I_6 + 0.13\ ^3H_6$
61	Γ_1		10722	$99.23\ ^1G_4 + 0.23\ ^1I_6 + 0.19\ ^3H_6$
62	Γ_2		10873	$98.81\ ^1G_4 + 0.49\ ^3F_4 + 0.24\ ^3H_6$
63	Γ_1		11010	$98.49\ ^1G_4 + 0.94\ ^3F_4 + 0.27\ ^1I_6$
64	Γ_2	$^1D_2$	16651	$98.71\ ^1D_2 + 0.67\ ^1I_6 + 0.18\ ^3P_2$
65	Γ_1	16840	17156	$99.04\ ^1D_2 + 0.41\ ^1I_6 + 0.24\ ^1G_4$
66	Γ_1		17467	$98.99\ ^1D_2 + 0.84\ ^1I_6 + 0.05\ ^1G_4$
67	Γ_2		17494	$98.47\ ^1D_2 + 0.95\ ^1I_6 + 0.20\ ^3P_1$
68	Γ_1		17943	$98.72\ ^1D_2 + 0.91\ ^1I_6 + 0.13\ ^3P_2$
69	Γ_1	$^3P_0$	20934	$99.19\ ^1I_6 + 0.44\ ^1D_2 + 0.15\ ^1G_4$
70	Γ_1	20706	20944	$99.06\ ^1I_6 + 0.45\ ^1D_2 + 0.17\ ^1G_4$
71	Γ_2	$^3P_1$	21178	$99.33\ ^1I_6 + 0.23\ ^1D_2 + 0.16\ ^1G_4$
72	Γ_1	21330	21194	$94.00\ ^3P_0 + 5.19\ ^3P_2 + 0.33\ ^1I_6$
73	Γ_2	$^1I_6$	21199	$99.25\ ^1I_6 + 0.29\ ^1D_2 + 0.15\ ^3P_1$
74	Γ_2	21500	21613	$90.85\ ^3P_1 + 8.35\ ^3P_2 + 0.35\ ^1I_6$
75	Γ_2	$^3P_2$	21662	$88.68\ ^3P_1 + 9.64\ ^3P_2 + 1.21\ ^1I_6$
76	Γ_1	22535	21951	$99.68\ ^1I_6 + 0.11\ ^1G_4 + 0.06\ ^3P_2$
77	Γ_1		22007	$98.80\ ^1I_6 + 0.47\ ^3P_2 + 0.29\ ^1D_2$
78	Γ_1		22190	$98.89\ ^3P_1 + 0.37\ ^3P_2 + 0.36\ ^1I_6$
79	Γ_2		22232	$99.26\ ^1I_6 + 0.37\ ^3P_1 + 0.14\ ^1D_2$
80	Γ_2		22341	$96.22\ ^1I_6 + 1.55\ ^3P_1 + 1.39\ ^3P_2$
81	Γ_1		22450	$98.11\ ^1I_6 + 1.02\ ^3P_2 + 0.36\ ^1D_2$
82	Γ_2		22634	$92.41\ ^1I_6 + 5.86\ ^3P_2 + 1.26\ ^3P_1$
83	Γ_1		22638	$89.75\ ^1I_6 + 9.10\ ^3P_2 + 0.75\ ^3P_0$
84	Γ_1		22959	$85.44\ ^3P_2 + 9.72\ ^1I_6 + 4.37\ ^3P_0$
85	Γ_2		22978	$78.21\ ^3P_2 + 14.25\ ^1I_6 + 6.94\ ^3P_1$
86	Γ_1		23071	$93.59\ ^1I_6 + 5.77\ ^3P_2 + 0.26\ ^1G_4$
87	Γ_2		23076	$85.26\ ^1I_6 + 13.15\ ^3P_2 + 1.16\ ^3P_1$
88	Γ_2		23216	$82.15\ ^3P_2 + 9.76\ ^1I_6 + 7.90\ ^3P_1$
89	Γ_1		23409	$93.26\ ^3P_2 + 6.22\ ^1I_6 + 0.15\ ^3P_0$
90	Γ_1		23457	$97.98\ ^3P_2 + 1.34\ ^1I_6 + 0.26\ ^3P_1$
91	Γ_1	$^1S_0$ 469001	47471	$99.85\ ^1S_0 + 0.05\ ^1G_4 + 0.05\ ^1D_2$

^{a}Aqueous centroids (cm^{-1}).

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^4I_{9/2}$	0	$98.91\ ^4I_{9/2} + 0.94\ ^4I_{11/2} + 0.05\ ^4I_{13/2}$
2	130	205	$98.67\ ^4I_{9/2} + 1.09\ ^4I_{11/2} + 0.10\ ^4I_{13/2}$
3		320	$98.13\ ^4I_{9/2} + 1.68\ ^4I_{11/2} + 0.07\ ^4I_{13/2}$
4		451	$98.99\ ^4I_{9/2} + 0.76\ ^4I_{11/2} + 0.10\ ^4I_{13/2}$
5		647	$98.64\ ^4I_{9/2} + 1.12\ ^4I_{11/2} + 0.09\ ^4I_{13/2}$
6	$^4I_{11/2}$	1977	$98.15\ ^4I_{11/2} + 0.94\ ^4I_{9/2} + 0.77\ ^4I_{13/2}$
7	2006	2121	$97.61\ ^4I_{11/2} + 1.56\ ^4I_{13/2} + 0.64\ ^4I_{9/2}$
8		2153	$98.08\ ^4I_{11/2} + 0.96\ ^4I_{9/2} + 0.84\ ^4I_{13/2}$
9		2311	$98.12\ ^4I_{11/2} + 0.89\ ^4I_{13/2} + 0.75\ ^4I_{9/2}$
10		2346	$97.72\ ^4I_{11/2} + 1.30\ ^4I_{9/2} + 0.79\ ^4I_{13/2}$
11		2443	$97.91\ ^4I_{11/2} + 1.03\ ^4I_{9/2} + 0.87\ ^4I_{13/2}$

Table 26 (cont'd).
Predicted energy
levels for Nd^{3+} in
$Ca_5(PO_4)_3F$, C_s site.
B_{nm} from table 9.

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
12	$^4I_{13/2}$	3946	$98.36\,^4I_{13/2} + 0.96\,^4I_{11/2} + 0.52\,^4I_{15/2}$
13	4004	4075	$97.75\,^4I_{13/2} + 1.16\,^4I_{15/2} + 0.88\,^4I_{11/2}$
14		4119	$98.57\,^4I_{13/2} + 0.86\,^4I_{15/2} + 0.41\,^4I_{11/2}$
15		4270	$97.70\,^4I_{13/2} + 1.06\,^4I_{15/2} + 1.03\,^4I_{11/2}$
16		4325	$98.55\,^4I_{13/2} + 0.86\,^4I_{15/2} + 0.45\,^4I_{11/2}$
17		4394	$97.74\,^4I_{13/2} + 1.34\,^4I_{11/2} + 0.79\,^4I_{15/2}$
18		4491	$98.53\,^4I_{13/2} + 0.72\,^4I_{11/2} + 0.54\,^4I_{15/2}$
19	$^4I_{15/2}$	5913	$98.82\,^4I_{15/2} + 1.01\,^4I_{13/2} + 0.06\,^4I_{11/2}$
20	6080	6026	$98.66\,^4I_{15/2} + 1.03\,^4I_{13/2} + 0.13\,^4F_{9/2}$
21		6112	$99.11\,^4I_{15/2} + 0.64\,^4I_{13/2} + 0.08\,^4F_{9/2}$
22		6315	$99.19\,^4I_{15/2} + 0.56\,^4I_{13/2} + 0.08\,^4F_{9/2}$
23		6381	$99.31\,^4I_{15/2} + 0.47\,^4I_{13/2} + 0.07\,^4F_{9/2}$
24		6515	$99.27\,^4I_{15/2} + 0.60\,^4I_{13/2} + 0.05\,^4I_{11/2}$
25		6576	$98.88\,^4I_{15/2} + 0.97\,^4I_{13/2} + 0.03\,^4F_{9/2}$
26		6722	$99.24\,^4I_{15/2} + 0.53\,^4I_{13/2} + 0.05\,^4F_{9/2}$
27	$^4F_{3/2}$	11604	$96.26\,^4F_{3/2} + 2.55\,^4F_{5/2} + 0.48\,^4F_{7/2}$
28	11526	11793	$94.10\,^4F_{3/2} + 3.23\,^4F_{5/2} + 1.07\,^4F_{7/2}$
29	$^4F_{5/2}$	12629	$87.38\,^4F_{5/2} + 8.42\,^2H_{9/2} + 2.39\,^4F_{7/2}$
30	12573	12716	$51.76\,^4F_{5/2} + 45.13\,^2H_{9/2} + 1.43\,^4F_{7/2}$
31	$^2H_{9/2}$	12846	$58.98\,^2H_{9/2} + 36.39\,^4F_{5/2} + 2.41\,^4F_{3/2}$
32	12738	12888	$61.71\,^4F_{5/2} + 34.38\,^2H_{9/2} + 1.53\,^4F_{7/2}$
33		12912	$86.46\,^2H_{9/2} + 11.78\,^4F_{5/2} + 0.84\,^4F_{7/2}$
34		12999	$78.68\,^2H_{9/2} + 18.52\,^4F_{5/2} + 2.02\,^4F_{7/2}$
35		13058	$89.25\,^2H_{9/2} + 9.26\,^4F_{5/2} + 0.87\,^4F_{7/2}$
36		13171	$91.52\,^2H_{9/2} + 6.89\,^4F_{5/2} + 0.72\,^4F_{7/2}$
37	$^4S_{3/2}$	13643	$75.54\,^4S_{3/2} + 21.69\,^4F_{7/2} + 0.84\,^4G_{5/2}$
38	13459	13668	$48.60\,^4S_{3/2} + 47.61\,^4F_{7/2} + 1.63\,^4F_{5/2}$
39	$^4F_{7/2}$	13701	$63.83\,^4S_{3/2} + 33.45\,^4F_{7/2} + 1.10\,^4F_{5/2}$
40	13564	13731	$86.22\,^4F_{7/2} + 8.61\,^4S_{3/2} + 1.94\,^4F_{9/2}$
41		13838	$92.54\,^4F_{7/2} + 3.26\,^4F_{9/2} + 1.80\,^4F_{5/2}$
42		14014	$95.38\,^4F_{7/2} + 1.42\,^4F_{5/2} + 1.22\,^4F_{9/2}$
43	$^4F_{9/2}$	14930	$96.81\,^4F_{9/2} + 1.78\,^4F_{7/2} + 0.62\,^4F_{5/2}$
44	14854	14975	$98.08\,^4F_{9/2} + 0.77\,^2H_{11/2} + 0.51\,^4F_{7/2}$
45		15082	$95.06\,^4F_{9/2} + 3.20\,^4F_{7/2} + 1.04\,^2H_{11/2}$
46		15266	$97.10\,^4F_{9/2} + 1.26\,^4F_{7/2} + 0.87\,^2H_{11/2}$
47		15321	$97.24\,^4F_{9/2} + 1.23\,^2H_{11/2} + 0.50\,^2G_{7/2}$
48	$^2H_{11/2}$	16234	$98.87\,^2H_{11/2} + 0.52\,^2G_{7/2} + 0.46\,^4F_{9/2}$
49	16043	16260	$99.04\,^2H_{11/2} + 0.30\,^2G_{7/2} + 0.24\,^4F_{9/2}$
50		16279	$98.06\,^2H_{11/2} + 0.94\,^4F_{9/2} + 0.44\,^2G_{7/2}$
51		16310	$98.56\,^2H_{11/2} + 0.64\,^4F_{9/2} + 0.37\,^2G_{7/2}$
52		16336	$98.65\,^2H_{11/2} + 0.87\,^4F_{9/2} + 0.17\,^2G_{7/2}$
53		16342	$98.43\,^2H_{11/2} + 0.92\,^4F_{9/2} + 0.38\,^2G_{7/2}$
54	$^4G_{5/2}$	17130	$84.61\,^4G_{5/2} + 13.55\,^2G_{7/2} + 0.54\,^4F_{7/2}$
55	17167	17357	$62.16\,^4G_{5/2} + 36.49\,^2G_{7/2} + 0.43\,^4F_{3/2}$
56	$^2G_{7/2}$	17486	$56.90\,^2G_{7/2} + 41.36\,^4G_{5/2} + 0.53\,^4F_{9/2}$
57	17334	17589	$96.54\,^2G_{7/2} + 1.94\,^4G_{5/2} + 0.63\,^2H_{11/2}$
58		17682	$84.44\,^2G_{7/2} + 14.31\,^4G_{5/2} + 0.54\,^2H_{11/2}$
59		17780	$66.26\,^2G_{7/2} + 32.20\,^4G_{5/2} + 0.38\,^4S_{3/2}$
60		17873	$59.11\,^4G_{5/2} + 40.05\,^2G_{7/2} + 0.24\,^4S_{3/2}$

^{a}Aqueous centroids (cm^{-1}).

Table 27. Predicted energy levels for Pm^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]$[a]	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^5I_4$	0	$99.07\ ^5I_4 + 0.70\ ^5I_5 + 0.18\ ^5I_6$
2	Γ_2	99	39	$98.30\ ^5I_4 + 1.51\ ^5I_5 + 0.12\ ^5I_6$
3	Γ_2		190	$97.68\ ^5I_4 + 2.08\ ^5I_5 + 0.19\ ^5I_6$
4	Γ_1		193	$99.36\ ^5I_4 + 0.45\ ^5I_5 + 0.13\ ^5I_6$
5	Γ_2		286	$98.07\ ^5I_4 + 1.69\ ^5I_5 + 0.14\ ^5I_6$
6	Γ_1		325	$98.30\ ^5I_4 + 1.42\ ^5I_5 + 0.25\ ^5I_6$
7	Γ_2		416	$98.53\ ^5I_4 + 1.27\ ^5I_5 + 0.11\ ^5I_6$
8	Γ_1		488	$95.19\ ^5I_4 + 4.57\ ^5I_5 + 0.18\ ^5I_6$
9	Γ_1		560	$97.73\ ^5I_4 + 1.94\ ^5I_5 + 0.26\ ^5I_6$
10	Γ_2	$^5I_5$	1642	$96.36\ ^5I_5 + 2.22\ ^5I_4 + 1.24\ ^5I_6$
11	Γ_1	1577	1645	$97.03\ ^5I_5 + 1.92\ ^5I_4 + 0.82\ ^5I_6$
12	Γ_2		1695	$98.27\ ^5I_5 + 0.88\ ^5I_4 + 0.57\ ^5I_6$
13	Γ_1		1697	$97.27\ ^5I_5 + 2.27\ ^5I_4 + 0.30\ ^5I_6$
14	Γ_2		1742	$97.92\ ^5I_5 + 1.34\ ^5I_4 + 0.42\ ^5I_6$
15	Γ_2		1796	$98.62\ ^5I_5 + 0.99\ ^5I_6 + 0.28\ ^5I_4$
16	Γ_1		1802	$97.10\ ^5I_5 + 1.77\ ^5I_6 + 1.00\ ^5I_4$
17	Γ_1		1813	$95.92\ ^5I_5 + 2.44\ ^5I_4 + 1.37\ ^5I_6$
18	Γ_1		1831	$96.52\ ^5I_5 + 1.84\ ^5I_6 + 1.43\ ^5I_4$
19	Γ_2		1966	$97.21\ ^5I_5 + 1.88\ ^5I_6 + 0.71\ ^5I_4$
20	Γ_2		1972	$97.18\ ^5I_5 + 1.53\ ^5I_6 + 1.03\ ^5I_4$
21	Γ_1	$^5I_6$	3245	$97.78\ ^5I_6 + 0.97\ ^5I_7 + 0.76\ ^5I_5$
22	Γ_2	3186	3259	$96.56\ ^5I_6 + 1.77\ ^5I_5 + 1.26\ ^5I_7$
23	Γ_2		3289	$98.59\ ^5I_6 + 0.63\ ^5I_5 + 0.47\ ^5I_7$
24	Γ_1		3307	$97.86\ ^5I_6 + 1.50\ ^5I_5 + 0.43\ ^5I_7$
25	Γ_2		3344	$97.96\ ^5I_6 + 1.46\ ^5I_5 + 0.37\ ^5I_7$
26	Γ_1		3357	$98.19\ ^5I_6 + 0.82\ ^5I_5 + 0.65\ ^5I_7$
27	Γ_1		3365	$97.02\ ^5I_6 + 1.33\ ^5I_7 + 1.28\ ^5I_5$
28	Γ_2		3424	$98.18\ ^5I_6 + 0.91\ ^5I_5 + 0.71\ ^5I_7$
29	Γ_1		3431	$98.34\ ^5I_6 + 0.98\ ^5I_7 + 0.44\ ^5I_5$
30	Γ_2		3448	$96.48\ ^5I_6 + 2.14\ ^5I_7 + 1.11\ ^5I_5$
31	Γ_2		3455	$97.32\ ^5I_6 + 1.93\ ^5I_7 + 0.58\ ^5I_5$
32	Γ_1		3587	$97.70\ ^5I_6 + 1.38\ ^5I_7 + 0.67\ ^5I_5$
33	Γ_1		3590	$98.01\ ^5I_6 + 1.14\ ^5I_7 + 0.58\ ^5I_5$
34	Γ_2	$^5I_7$	4902	$97.99\ ^5I_7 + 0.94\ ^5I_6 + 0.68\ ^5I_8$
35	Γ_1	4876	4903	$97.29\ ^5I_7 + 1.33\ ^5I_6 + 1.03\ ^5I_8$
36	Γ_2		4971	$98.83\ ^5I_7 + 0.54\ ^5I_8 + 0.47\ ^5I_6$
37	Γ_1		4983	$98.64\ ^5I_7 + 0.78\ ^5I_8 + 0.40\ ^5I_6$
38	Γ_1		4995	$98.21\ ^5I_7 + 0.87\ ^5I_6 + 0.69\ ^5I_8$
39	Γ_2		5013	$97.96\ ^5I_7 + 1.29\ ^5I_6 + 0.62\ ^5I_8$
40	Γ_1		5031	$97.45\ ^5I_7 + 1.85\ ^5I_6 + 0.59\ ^5I_8$
41	Γ_2		5062	$96.60\ ^5I_7 + 1.96\ ^5I_8 + 1.19\ ^5I_6$
42	Γ_2		5076	$97.70\ ^5I_7 + 1.10\ ^5I_8 + 1.02\ ^5I_6$
43	Γ_1		5143	$97.77\ ^5I_7 + 1.88\ ^5I_8 + 0.15\ ^5I_6$
44	Γ_2		5166	$98.46\ ^5I_7 + 0.75\ ^5I_8 + 0.59\ ^5I_6$
45	Γ_1		5185	$96.78\ ^5I_7 + 1.95\ ^5I_8 + 1.10\ ^5I_6$
46	Γ_1		5208	$98.16\ ^5I_7 + 1.10\ ^5I_6 + 0.63\ ^5I_8$
47	Γ_2		5323	$98.17\ ^5I_7 + 0.96\ ^5I_8 + 0.67\ ^5I_6$
48	Γ_2		5325	$98.39\ ^5I_7 + 0.80\ ^5I_8 + 0.60\ ^5I_6$

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
49	Γ_2	$^5I_8$	6502	$98.61\ ^5I_8 + 1.16\ ^5I_7 + 0.15\ ^5I_6$
50	Γ_1	6611	6506	$98.58\ ^5I_8 + 1.17\ ^5I_7 + 0.15\ ^5I_6$
51	Γ_1		6600	$98.92\ ^5I_8 + 0.95\ ^5I_7 + 0.07\ ^5I_6$
52	Γ_2		6667	$98.24\ ^5I_8 + 1.60\ ^5I_7 + 0.05\ ^5F_5$
53	Γ_1		6674	$99.08\ ^5I_8 + 0.79\ ^5I_7 + 0.07\ ^5I_6$
54	Γ_2		6686	$99.23\ ^5I_8 + 0.66\ ^5I_7 + 0.06\ ^5I_6$
55	Γ_2		6695	$98.53\ ^5I_8 + 1.32\ ^5I_7 + 0.06\ ^5I_6$
56	Γ_1		6769	$99.47\ ^5I_8 + 0.39\ ^5I_7 + 0.06\ ^5F_5$
57	Γ_2		6809	$99.36\ ^5I_8 + 0.45\ ^5I_7 + 0.07\ ^5F_5$
58	Γ_1		6825	$98.95\ ^5I_8 + 0.86\ ^5I_7 + 0.06\ ^5F_4$
59	Γ_1		6921	$97.98\ ^5I_8 + 1.77\ ^5I_7 + 0.11\ ^5F_5$
60	Γ_2		6997	$99.41\ ^5I_8 + 0.35\ ^5I_7 + 0.08\ ^5I_6$
61	Γ_1		7021	$99.21\ ^5I_8 + 0.57\ ^5I_7 + 0.09\ ^5F_5$
62	Γ_2		7068	$98.77\ ^5I_8 + 1.01\ ^5I_7 + 0.12\ ^5F_5$
63	Γ_2		7086	$98.95\ ^5I_8 + 0.81\ ^5I_7 + 0.11\ ^5F_5$
64	Γ_1		7188	$99.35\ ^5I_8 + 0.50\ ^5I_7 + 0.08\ ^5I_6$
65	Γ_1		7191	$99.39\ ^5I_8 + 0.45\ ^5I_7 + 0.08\ ^5I_6$
66	Γ_2	$^5F_1$	12501	$95.17\ ^5F_1 + 2.75\ ^5F_2 + 1.53\ ^5F_3$
67	Γ_2	12397	12523	$89.18\ ^5F_1 + 9.42\ ^5F_2 + 0.99\ ^5F_3$
68	Γ_1		12686	$91.74\ ^5F_1 + 4.60\ ^5F_2 + 3.14\ ^5F_3$
69	Γ_1	$^5F_2$	12799	$95.35\ ^5F_2 + 2.46\ ^5F_1 + 1.66\ ^5F_3$
70	Γ_2	12811	12976	$87.76\ ^5F_2 + 8.84\ ^5F_1 + 1.95\ ^5F_3$
71	Γ_1		12996	$94.54\ ^5F_2 + 2.66\ ^5F_1 + 2.19\ ^5F_3$
72	Γ_1		13069	$97.92\ ^5F_2 + 1.45\ ^5F_4 + 0.27\ ^5F_3$
73	Γ_2		13279	$93.11\ ^5F_2 + 2.99\ ^5F_3 + 2.97\ ^5F_1$
74	Γ_2	$^5F_3$	13727	$96.86\ ^5F_3 + 2.28\ ^5F_4 + 0.31\ ^5F_1$
75	Γ_2	13651	13744	$95.62\ ^5F_3 + 1.89\ ^5F_2 + 1.48\ ^5F_1$
76	Γ_1		13823	$94.53\ ^5F_3 + 2.78\ ^5F_4 + 1.84\ ^5F_2$
77	Γ_2		13827	$93.58\ ^5F_3 + 2.43\ ^5F_2 + 2.33\ ^5F_4$
78	Γ_1		13918	$93.41\ ^5F_3 + 4.35\ ^5F_4 + 1.31\ ^5F_2$
79	Γ_1		13987	$93.14\ ^5F_3 + 2.80\ ^5F_4 + 2.32\ ^5F_1$
80	Γ_2		14074	$96.57\ ^5F_3 + 2.40\ ^5F_4 + 0.45\ ^5F_2$
81	Γ_1	$^5S_2$	14550	$99.78\ ^5S_2 + 0.14\ ^5F_4 + 0.02\ ^5F_3$
82	Γ_2	14337	14552	$99.52\ ^5S_2 + 0.37\ ^5F_4 + 0.04\ ^5F_5$
83	Γ_1		14558	$99.58\ ^5S_2 + 0.27\ ^5F_4 + 0.06\ ^5F_5$
84	Γ_2		14559	$99.87\ ^5S_2 + 0.05\ ^5F_4 + 0.02\ ^5F_3$
85	Γ_1		14561	$99.70\ ^5S_2 + 0.15\ ^5F_4 + 0.06\ ^5F_5$
86	Γ_1	$^5F_4$	14714	$97.60\ ^5F_4 + 1.44\ ^5F_5 + 0.41\ ^5F_2$
87	Γ_2	14561	14728	$94.03\ ^5F_4 + 3.47\ ^5F_5 + 2.00\ ^5F_3$
88	Γ_1		14738	$95.69\ ^5F_4 + 1.92\ ^5F_5 + 1.65\ ^5F_3$
89	Γ_2		14767	$94.20\ ^5F_4 + 2.99\ ^5F_5 + 1.89\ ^5F_3$
90	Γ_1		14793	$93.50\ ^5F_4 + 4.94\ ^5F_3 + 1.16\ ^5F_5$
91	Γ_2		14853	$96.25\ ^5F_4 + 1.46\ ^5F_3 + 1.05\ ^5F_5$
92	Γ_1		14857	$96.12\ ^5F_4 + 3.09\ ^5F_3 + 0.48\ ^5F_5$
93	Γ_1		14865	$97.02\ ^5F_4 + 1.35\ ^5F_2 + 0.98\ ^5F_5$
94	Γ_2		14868	$96.38\ ^5F_4 + 2.53\ ^5F_3 + 0.43\ ^5F_5$
95	Γ_2	$^5F_5$	15865	$98.90\ ^5F_5 + 0.33\ ^3K_6 + 0.27\ ^5F_3$
96	Γ_2	15862	15874	$98.16\ ^5F_5 + 0.90\ ^5F_4 + 0.54\ ^3K_6$
97	Γ_1	$^3K_6$	15929	$96.69\ ^5F_5 + 1.83\ ^3K_6 + 0.91\ ^5F_4$

Table 27 (cont'd). Predicted energy levels for Pm^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Table 27 (cont'd). Predicted energy levels for Pm^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
98	Γ_1	15874	15940	$94.50\,^5F_5 + 3.20\,^3K_6 + 1.94\,^5F_4$
99	Γ_1		16025	$98.68\,^3K_6 + 1.28\,^5F_5 + 0.03\,^5F_4$
100	Γ_1		16026	$97.35\,^3K_6 + 2.62\,^5F_5 + 0.01\,^5F_4$
101	Γ_2		16065	$99.61\,^3K_6 + 0.36\,^5F_5 + 0.02\,^5F_4$
102	Γ_2		16067	$99.09\,^3K_6 + 0.86\,^5F_5 + 0.03\,^5F_3$
103	Γ_1		16079	$98.13\,^3K_6 + 1.71\,^5F_5 + 0.14\,^5F_4$
104	Γ_2		16080	$99.08\,^3K_6 + 0.83\,^5F_5 + 0.07\,^5F_4$
105	Γ_1		16101	$99.02\,^3K_6 + 0.95\,^5F_5 + 0.02\,^5F_3$
106	Γ_1		16101	$99.16\,^3K_6 + 0.79\,^5F_5 + 0.03\,^5F_4$
107	Γ_2		16111	$90.74\,^3K_6 + 9.06\,^5F_5 + 0.17\,^5F_4$
108	Γ_2		16120	$94.40\,^3K_6 + 5.39\,^5F_5 + 0.18\,^5F_4$
109	Γ_1		16120	$99.45\,^3K_6 + 0.52\,^5F_5 + 0.02\,^5F_3$
110	Γ_2		16135	$75.39\,^3K_6 + 23.65\,^5F_5 + 0.88\,^5F_4$
111	Γ_1		16143	$98.92\,^3K_6 + 1.00\,^5F_5 + 0.04\,^5F_4$
112	Γ_2		16151	$61.89\,^5F_5 + 36.02\,^3K_6 + 1.90\,^5F_4$
113	Γ_1		16173	$96.43\,^5F_5 + 1.88\,^3K_6 + 1.44\,^5F_4$
114	Γ_2		16210	$96.73\,^5F_5 + 2.13\,^5F_4 + 0.70\,^3K_6$
115	Γ_1		16218	$97.04\,^5F_5 + 1.59\,^3K_6 + 1.07\,^5F_4$
116	Γ_2		16238	$95.27\,^5F_5 + 3.55\,^3K_6 + 0.88\,^5F_4$
117	Γ_2		16347	$98.48\,^5F_5 + 0.70\,^5F_4 + 0.35\,^5F_3$
118	Γ_1		16349	$98.24\,^5F_5 + 0.79\,^5F_4 + 0.50\,^3K_6$

[a] Aqueous centroids (cm^{-1}).

Table 28. Predicted energy levels for Sm^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^6H_{5/2}$	0	$96.70\,^6H_{5/2} + 2.54\,^6H_{7/2} + 0.25\,^6H_{9/2}$
2	46	241	$94.54\,^6H_{5/2} + 4.17\,^6H_{7/2} + 0.84\,^6H_{9/2}$
3		509	$87.61\,^6H_{5/2} + 11.24\,^6H_{7/2} + 0.84\,^6H_{9/2}$
4	$^6H_{7/2}$	1135	$93.83\,^6H_{7/2} + 2.71\,^6H_{9/2} + 2.62\,^6H_{5/2}$
5	1084	1241	$93.81\,^6H_{7/2} + 3.25\,^6H_{5/2} + 1.81\,^6H_{9/2}$
6		1472	$84.91\,^6H_{7/2} + 8.89\,^6H_{5/2} + 5.16\,^6H_{9/2}$
7		1580	$91.58\,^6H_{7/2} + 5.47\,^6H_{9/2} + 2.19\,^6H_{5/2}$
8	$^6H_{9/2}$	2349	$94.81\,^6H_{9/2} + 2.32\,^6H_{11/2} + 1.62\,^6H_{7/2}$
9	2299	2449	$94.72\,^6H_{9/2} + 2.58\,^6H_{7/2} + 1.35\,^6H_{11/2}$
10		2549	$90.37\,^6H_{9/2} + 3.81\,^6H_{11/2} + 3.50\,^6H_{7/2}$
11		2712	$90.04\,^6H_{9/2} + 4.29\,^6H_{11/2} + 4.14\,^6H_{7/2}$
12		2811	$93.46\,^6H_{9/2} + 4.06\,^6H_{11/2} + 1.59\,^6H_{7/2}$
13	$^6H_{11/2}$	3653	$94.84\,^6H_{11/2} + 2.06\,^6H_{13/2} + 1.51\,^6H_{9/2}$
14	3638	3783	$95.60\,^6H_{11/2} + 1.67\,^6H_{13/2} + 1.29\,^6H_{9/2}$
15		3855	$91.64\,^6H_{11/2} + 4.08\,^6H_{9/2} + 2.53\,^6H_{13/2}$
16		3925	$92.37\,^6H_{11/2} + 2.79\,^6H_{9/2} + 2.78\,^6H_{13/2}$
17		4065	$90.51\,^6H_{11/2} + 4.70\,^6H_{13/2} + 3.56\,^6H_{9/2}$
18		4181	$93.36\,^6H_{11/2} + 4.79\,^6H_{13/2} + 1.04\,^6H_{9/2}$
19	$^6H_{13/2}$	4984	$95.39\,^6H_{13/2} + 1.31\,^6H_{15/2} + 1.16\,^6H_{11/2}$
20	5060	5178	$92.68\,^6H_{13/2} + 2.63\,^6H_{15/2} + 2.42\,^6H_{11/2}$
21		5257	$93.16\,^6H_{13/2} + 3.69\,^6H_{11/2} + 1.35\,^6H_{15/2}$
22		5300	$95.00\,^6H_{13/2} + 2.21\,^6H_{15/2} + 1.39\,^6H_{11/2}$
23		5385	$92.31\,^6H_{13/2} + 3.22\,^6H_{11/2} + 2.72\,^6H_{15/2}$
24		5513	$88.78\,^6H_{13/2} + 5.21\,^6H_{15/2} + 4.42\,^6H_{11/2}$
25		5715	$94.47\,^6H_{13/2} + 3.61\,^6H_{15/2} + 0.94\,^6H_{11/2}$

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
			Table 28 (cont'd). Predicted energy levels for Sm^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.
26	$^6F_{1/2}$	6326	$96.32\ ^6H_{15/2} + 0.96\ ^6F_{9/2} + 0.82\ ^6H_{13/2}$
27	6422	6467	$95.39\ ^6H_{15/2} + 1.83\ ^6H_{13/2} + 0.96\ ^6F_{11/2}$
28	$^6H_{15/2}$ 6531	6657	$92.85\ ^6H_{15/2} + 2.79\ ^6H_{13/2} + 1.82\ ^6F_{3/2}$
29	$^6F_{3/2}$	6698	$94.05\ ^6H_{15/2} + 3.04\ ^6H_{13/2} + 0.86\ ^6F_{7/2}$
30	6666	6744	$87.21\ ^6F_{1/2} + 7.87\ ^6F_{3/2} + 1.47\ ^6H_{15/2}$
31		6859	$91.58\ ^6H_{15/2} + 3.42\ ^6F_{3/2} + 2.57\ ^6H_{13/2}$
32		6972	$83.31\ ^6H_{15/2} + 11.40\ ^6F_{3/2} + 1.79\ ^6H_{13/2}$
33		7004	$72.34\ ^6F_{3/2} + 13.91\ ^6H_{15/2} + 6.51\ ^6F_{5/2}$
34		7038	$88.44\ ^6F_{3/2} + 3.64\ ^6F1/2 + 3.44\ ^6H_{15/2}$
35		7173	$91.25\ ^6H_{15/2} + 3.28\ ^6H_{13/2} + 2.92\ ^6F_{5/2}$
36		7437	$89.08\ ^6H_{15/2} + 7.35\ ^6F_{5/2} + 1.27\ ^6F_{7/2}$
37	$^6F_{5/2}$	7471	$89.61\ ^6F_{5/2} + 6.62\ ^6H_{15/2} + 0.84\ ^6F_{3/2}$
38	7158	7552	$89.25\ ^6F_{5/2} + 4.09\ ^6H_{15/2} + 3.14\ ^6F_{3/2}$
39		7618	$90.01\ ^6F_{5/2} + 4.67\ ^6F_{3/2} + 1.87\ ^6H_{15/2}$
40	$^6F_{7/2}$	8303	$96.12\ ^6F_{7/2} + 1.77\ ^6H_{15/2} + 0.66\ ^6H_{13/2}$
41	8006	8327	$96.74\ ^6F_{7/2} + 0.66\ ^6F_{9/2} + 0.63\ ^6H_{13/2}$
42		8416	$95.05\ ^6F_{7/2} + 1.35\ ^6F_{5/2} + 1.12\ ^6H_{15/2}$
43		8495	$95.54\ ^6F_{7/2} + 1.53\ ^6H_{15/2} + 0.65\ ^6H_{13/2}$
44	$^6F_{9/2}$	9418	$97.78\ ^6F_{9/2} + 1.18\ ^6H_{15/2} + 0.43\ ^6F_{7/2}$
45	9167	9506	$96.60\ ^6F_{9/2} + 1.31\ ^6F_{11/2} + 0.67\ ^6H_{15/2}$
46		9541	$95.80\ ^6F_{9/2} + 1.92\ ^6F_{11/2} + 0.68\ ^6H_{15/2}$
47		9604	$97.44\ ^6F_{9/2} + 1.10\ ^6H_{15/2} + 0.38\ ^6H_{13/2}$
48		9630	$97.11\ ^6F_{9/2} + 0.94\ ^6H_{15/2} + 0.64\ ^6F_{7/2}$
49	$^6F_{11/2}$	10742	$98.57\ ^6F_{11/2} + 0.77\ ^6H_{15/2} + 0.26\ ^6F_{9/2}$
50	10552	10798	$98.51\ ^6F_{11/2} + 0.42\ ^6H_{13/2} + 0.41\ ^6H_{15/2}$
51		10943	$97.43\ ^6F_{11/2} + 1.12\ ^6F_{9/2} + 0.92\ ^6H_{15/2}$
52		10980	$98.80\ ^6F_{11/2} + 0.48\ ^6F_{9/2} + 0.42\ ^6H_{15/2}$
53		10988	$97.76\ ^6F_{11/2} + 1.08\ ^6F_{9/2} + 0.70\ ^6H_{15/2}$
54		11125	$97.37\ ^6F_{11/2} + 1.78\ ^6H_{15/2} + 0.33\ ^6H_{13/2}$
55	$^4G_{5/2}$	17857	$98.44\ ^4G_{5/2} + 1.55\ ^4F_{3/2}$
56	17935	18234	$97.84\ ^4G_{5/2} + 2.16\ ^4F_{3/2}$
57		18597	$98.86\ ^4G_{5/2} + 1.14\ ^4F_{3/2}$
58	$^4F_{3/2}$	19211	$98.18\ ^4F_{3/2} + 1.82\ ^4G_{5/2}$
59	18899	19261	$96.97\ ^4F_{3/2} + 3.03\ ^4G_{5/2}$

^{a}Aqueous centroids (cm^{-1}).

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
				Table 29. Predicted energy levels for Eu^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.
1	Γ_1	$^7F_0$	0	$91.81\ ^7F_0 + 6.51\ ^7F_2 + 1.56\ ^7F_4$
2	Γ_2	$^7F_1$	252	$95.54\ ^7F_1 + 1.82\ ^7F_3 + 1.35\ ^7F_2$
3	Γ_2	354	288	$92.28\ ^7F_1 + 3.93\ ^7F_3 + 2.71\ ^7F_2$
4	Γ_1		670	$89.80\ ^7F_1 + 5.46\ ^7F_3 + 3.44\ ^7F_2$
5	Γ_1	$^7F_2$	819	$91.25\ ^7F_2 + 5.93\ ^7F_3 + 1.49\ ^7F_1$
6	Γ_1	1018	919	$85.02\ ^7F_2 + 11.01\ ^7F_3 + 2.49\ ^7F_1$
7	Γ_2		1065	$93.35\ ^7F_2 + 2.66\ ^7F_1 + 1.51\ ^7F_5$
8	Γ_1		1258	$87.02\ ^7F_2 + 5.12\ ^7F_0 + 4.73\ ^7F_3$
9	Γ_2		1384	$80.73\ ^7F_2 + 16.47\ ^7F_3 + 1.67\ ^7F_4$

	Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
Table 29 (cont'd). Predicted energy levels for Eu^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.	10	Γ_2	$^7F_3$	1823	$91.05\,^7F_3 + 6.67\,^7F_4 + 1.06\,^7F_5$
	11	Γ_2	1881	1911	$77.28\,^7F_3 + 12.51\,^7F_2 + 8.94\,^7F_4$
	12	Γ_1		1963	$79.43\,^7F_3 + 10.43\,^7F_4 + 8.37\,^7F_2$
	13	Γ_1		2077	$90.54\,^7F_3 + 3.54\,^7F_1 + 3.31\,^7F_5$
	14	Γ_2		2085	$90.82\,^7F_3 + 3.93\,^7F_2 + 3.50\,^7F_5$
	15	Γ_1		2114	$74.11\,^7F_3 + 13.83\,^7F_4 + 9.92\,^7F_2$
	16	Γ_2		2133	$89.66\,^7F_3 + 5.35\,^7F_1 + 3.97\,^7F_4$
	17	Γ_1	$^7F_4$	2764	$84.91\,^7F_4 + 8.45\,^7F_3 + 3.21\,^7F_5$
	18	Γ_2	2867	2772	$94.17\,^7F_4 + 2.44\,^7F_5 + 1.30\,^7F_3$
	19	Γ_2		2934	$84.96\,^7F_4 + 7.07\,^7F_5 + 4.85\,^7F_3$
	20	Γ_1		2937	$78.74\,^7F_4 + 12.21\,^7F_3 + 5.82\,^7F_5$
	21	Γ_1		3091	$92.30\,^7F_4 + 3.22\,^7F_5 + 2.53\,^7F_6$
	22	Γ_2		3101	$84.81\,^7F_4 + 8.81\,^7F_3 + 4.55\,^7F_5$
	23	Γ_1		3174	$88.56\,^7F_4 + 8.03\,^7F_5 + 1.71\,^7F_6$
	24	Γ_1		3208	$90.44\,^7F_4 + 4.77\,^7F_5 + 2.08\,^7F_6$
	25	Γ_2		3230	$87.37\,^7F_4 + 5.89\,^7F_5 + 3.79\,^7F_3$
	26	Γ_1	$^7F_5$	3858	$86.02\,^7F_5 + 10.09\,^7F_6 + 2.71\,^7F_4$
	27	Γ_2	3928	3875	$83.05\,^7F_5 + 10.16\,^7F_6 + 4.50\,^7F_4$
	28	Γ_2		3892	$85.02\,^7F_5 + 8.73\,^7F_6 + 4.88\,^7F_4$
	29	Γ_1		3921	$86.95\,^7F_5 + 7.19\,^7F_6 + 4.83\,^7F_4$
	30	Γ_2		3977	$89.33\,^7F_5 + 7.54\,^7F_6 + 2.00\,^7F_4$
	31	Γ_1		3986	$87.03\,^7F_5 + 8.56\,^7F_6 + 1.86\,^7F_3$
	32	Γ_2		4121	$90.83\,^7F_5 + 3.05\,^7F_6 + 2.99\,^7F_3$
	33	Γ_1		4148	$83.94\,^7F_5 + 7.83\,^7F_4 + 7.14\,^7F_6$
	34	Γ_1		4290	$86.19\,^7F_5 + 7.86\,^7F_4 + 4.44\,^7F_6$
	35	Γ_2		4437	$93.69\,^7F_5 + 4.60\,^7F_6 + 0.88\,^7F_4$
	36	Γ_2		4463	$95.34\,^7F_5 + 2.57\,^7F_6 + 1.47\,^7F_4$
	37	Γ_1	$^7F_6$	4908	$91.27\,^7F_6 + 4.38\,^7F_5 + 3.66\,^7F_4$
	38	Γ_2	5029	4908	$90.66\,^7F_6 + 4.84\,^7F_5 + 3.92\,^7F_4$
	39	Γ_1		4951	$96.59\,^7F_6 + 1.72\,^7F_5 + 1.47\,^7F_4$
	40	Γ_2		4955	$95.71\,^7F_6 + 2.96\,^7F_5 + 0.88\,^7F_4$
	41	Γ_1		5162	$90.70\,^7F_6 + 6.69\,^7F_5 + 1.99\,^7F_4$
	42	Γ_2		5201	$90.80\,^7F_6 + 7.80\,^7F_5 + 0.79\,^7F_4$
	43	Γ_2		5321	$85.27\,^7F_6 + 13.49\,^7F_5 + 0.94\,^7F_4$
	44	Γ_1		5409	$89.29\,^7F_6 + 9.68\,^7F_5 + 0.91\,^7F_4$
	45	Γ_1		5447	$86.94\,^7F_6 + 12.83\,^7F_5 + 0.14\,^7F_4$
	46	Γ_2		5611	$96.66\,^7F_6 + 2.63\,^7F_5 + 0.47\,^7F_4$
	47	Γ_2		5617	$96.53\,^7F_6 + 2.83\,^7F_5 + 0.37\,^7F_4$
	48	Γ_1		5719	$98.33\,^7F_6 + 1.05\,^7F_5 + 0.54\,^7F_4$
	49	Γ_1		5720	$98.42\,^7F_6 + 0.95\,^7F_5 + 0.55\,^7F_4$
	50	Γ_1	$^5D_0$ 17286	17447	$99.89\,^5D_0 + 0.06\,^5D_2 + 0.05\,^5L_6$
	51	Γ_2	$^5D_1$	19135	$99.91\,^5D_1 + 0.05\,^5D_2 + 0.03\,^5D_3$
	52	Γ_2	19026	19167	$99.89\,^5D_1 + 0.09\,^5D_2 + 0.02\,^5L_6$
	53	Γ_1		19270	$99.94\,^5D_1 + 0.04\,^5D_3 + 0.02\,^5L_6$
	54	Γ_2	$^5D_2$	21619	$99.78\,^5D_2 + 0.13\,^5D_3 + 0.05\,^5D_1$
	55	Γ_1	21499	21626	$99.85\,^5D_2 + 0.10\,^5D_3 + 0.03\,^5L_6$
	56	Γ_1		21649	$99.81\,^5D_2 + 0.14\,^5D_3 + 0.03\,^5L_6$
	57	Γ_2		21696	$99.77\,^5D_2 + 0.10\,^5D_3 + 0.09\,^5D_1$
	58	Γ_1		21728	$99.94\,^5D_2 + 0.03\,^5D_0 + 0.02\,^5L_6$

Table 29 (cont'd). Predicted energy levels for Eu^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
59	Γ_1	$^5D_3$	24504	99.87 $^5D_3$ + 0.06 $^5D_2$ + 0.04 $^5L_6$
60	Γ_2	24390	24514	99.85 $^5D_3$ + 0.09 $^5D_2$ + 0.03 $^5L_6$
61	Γ_2		24523	99.88 $^5D_3$ + 0.10 $^5D_2$ + 0.02 $^5L_6$
62	Γ_1		24560	99.87 $^5D_3$ + 0.07 $^5L_6$ + 0.06 $^5D_2$
63	Γ_1		24581	99.83 $^5D_3$ + 0.13 $^5D_2$ + 0.04 $^5L_6$
64	Γ_2		24610	99.92 $^5D_3$ + 0.04 $^5L_6$ + 0.04 $^5D_2$
65	Γ_2		24626	99.96 $^5D_3$ + 0.03 $^5L_6$ + 0.01 $^5D_1$
66	Γ_1	$^5L_6$	25171	99.90 $^5L_6$ + 0.06 $^5D_3$ + 0.02 $^5D_2$
67	Γ_2	25375	25201	99.93 $^5L_6$ + 0.04 $^5D_3$ + 0.02 $^5D_2$
68	Γ_1		25214	99.93 $^5L_6$ + 0.04 $^5D_3$ + 0.02 $^5D_2$
69	Γ_2		25246	99.96 $^5L_6$ + 0.01 $^5D_2$ + 0.01 $^5D_3$
70	Γ_2		25407	99.96 $^5L_6$ + 0.02 $^5D_3$ + 0.01 $^5D_2$
71	Γ_1		25436	99.96 $^5L_6$ + 0.03 $^5D_3$ + 0.01 $^5D_2$
72	Γ_1		25509	99.98 $^5L_6$ + 0.01 $^5D_0$ + 0.01 $^5D_2$
73	Γ_2		25656	99.96 $^5L_6$ + 0.02 $^5D_3$ + 0.01 $^5D_2$
74	Γ_2		25718	99.98 $^5L_6$ + 0.01 $^5D_2$ + 0.01 $^5D_3$
75	Γ_1		25835	99.98 $^5L_6$ + 0.01 $^5D_0$ + 0.01 $^5D_3$
76	Γ_1		25856	99.98 $^5L_6$ + 0.01 $^5D_2$
77	Γ_1		25908	99.97 $^5L_6$ + 0.02 $^5D_2$ + 0.01 $^5D_3$
78	Γ_2		25915	99.96 $^5L_6$ + 0.02 $^5D_3$ + 0.02 $^5D_2$

^{a}Aqueous centroids (cm^{-1}).

Table 30. Predicted energy levels for Gd^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^8S_{7/2}$	0	100.00 $^8S_{7/2}$
2	14	0.3	100.00 $^8S_{7/2}$
3		0.8	100.00 $^8S_{7/2}$
4		1.4	100.00 $^8S_{7/2}$
5	$^6P_{7/2}$	32074	99.44 $^6P_{7/2}$ + 0.15 $^6P_{3/2}$ + 0.09 $^6P_{5/2}$
6	32224	32127	98.84 $^6P_{7/2}$ + 0.69 $^6P_{5/2}$ + 0.15 $^6P_{3/2}$
7		32217	98.59 $^6P_{7/2}$ + 1.06 $^6P_{5/2}$ + 0.07 $^6I_{13/2}$
8		32340	99.54 $^6P_{7/2}$ + 0.08 $^6I_{17/2}$ + 0.06 $^6I_{11/2}$
9	$^6P_{5/2}$	32661	98.30 $^6P_{5/2}$ + 0.78 $^6P_{3/2}$ + 0.40 $^6P_{7/2}$
10	32767	32706	95.08 $^6P_{5/2}$ + 3.74 $^6P_{3/2}$ + 0.73 $^6P_{7/2}$
11		32815	98.55 $^6P_{5/2}$ + 0.82 $^6P_{7/2}$ + 0.16 $^6I_{17/2}$
12	$^6P_{3/2}$	33247	95.61 $^6P_{3/2}$ + 3.74 $^6P_{5/2}$ + 0.13 $^6I_{13/2}$
13	33303	33319	98.30 $^6P_{3/2}$ + 1.01 $^6P_{5/2}$ + 0.14 $^6I_{13/2}$
14	$^6I_{7/2}$	35823	99.54 $^6I_{7/2}$ + 0.21 $^6I_{9/2}$ + 0.13 $^6P_{5/2}$
15	35879	35841	99.77 $^6I_{7/2}$ + 0.17 $^6I_{9/2}$ + 0.01 $^6P_{7/2}$
16		35890	99.49 $^6I_{7/2}$ + 0.28 $^6I_{9/2}$ + 0.13 $^6P_{5/2}$
17		35917	99.52 $^6I_{7/2}$ + 0.24 $^6I_{9/2}$ + 0.13 $^6P_{5/2}$
18	$^6I_{9/2}$	36164	99.09 $^6I_{9/2}$ + 0.28 $^6I_{11/2}$ + 0.18 $^6I_{13/2}$
19	36231	36185	99.36 $^6I_{9/2}$ + 0.30 $^6I_{11/2}$ + 0.17 $^6I_{7/2}$
20		36206	98.77 $^6I_{9/2}$ + 0.64 $^6I_{11/2}$ + 0.22 $^6I_{7/2}$
21		36261	98.95 $^6I_{9/2}$ + 0.42 $^6I_{11/2}$ + 0.18 $^6I_{7/2}$
22		36278	98.77 $^6I_{9/2}$ + 0.58 $^6I_{11/2}$ + 0.15 $^6I_{15/2}$

	Table 30 (cont'd). Predicted energy levels for Gd^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
23	$^6I_{17/2}$	36433	$67.66\ ^6I_{17/2} + 29.81\ ^6I_{11/2} + 1.19\ ^6I_{15/2}$
24	36462	36441	$86.79\ ^6I_{17/2} + 10.77\ ^6I_{11/2} + 1.35\ ^6I_{13/2}$
25		36443	$93.57\ ^6I_{17/2} + 3.69\ ^6I_{11/2} + 2.05\ ^6I_{15/2}$
26		36444	$96.25\ ^6I_{17/2} + 2.07\ ^6I_{11/2} + 1.40\ ^6I_{15/2}$
27		36445	$94.20\ ^6I_{17/2} + 4.08\ ^6I_{11/2} + 0.91\ ^6I_{15/2}$
28		36446	$97.16\ ^6I_{17/2} + 1.66\ ^6I_{15/2} + 0.53\ ^6I_{11/2}$
29		36447	$96.36\ ^6I_{17/2} + 2.46\ ^6I_{11/2} + 0.61\ ^6I_{13/2}$
30		36449	$93.64\ ^6I_{17/2} + 4.81\ ^6I_{11/2} + 0.90\ ^6I_{15/2}$
31		36450	$97.62\ ^6I_{17/2} + 0.96\ ^6I_{11/2} + 0.74\ ^6I_{15/2}$
32	$^6I_{11/2}$	36459	$54.77\ ^6I_{11/2} + 42.19\ ^6I_{17/2} + 2.43\ ^6I_{15/2}$
33	36526	36478	$95.57\ ^6I_{11/2} + 3.00\ ^6I_{17/2} + 0.71\ ^6I_{13/2}$
34		36495	$91.18\ ^6I_{11/2} + 6.30\ ^6I_{17/2} + 1.53\ ^6I_{13/2}$
35		36514	$92.91\ ^6I_{11/2} + 4.95\ ^6I_{17/2} + 0.89\ ^6I_{13/2}$
36		36567	$95.23\ ^6I_{11/2} + 1.54\ ^6I_{13/2} + 1.41\ ^6I_{17/2}$
37		36579	$94.45\ ^6I_{11/2} + 2.05\ ^6I_{15/2} + 1.71\ ^6I_{17/2}$
38	$^6I_{13/2}$	36636	$92.62\ ^6I_{13/2} + 3.89\ ^6I_{15/2} + 2.32\ ^6I_{17/2}$
39	36711	36655	$71.13\ ^6I_{13/2} + 25.86\ ^6I_{15/2} + 1.98\ ^6I_{11/2}$
40	$^6I_{15/2}$	36658	$55.23\ ^6I_{13/2} + 42.27\ ^6I_{15/2} + 1.44\ ^6I_{11/2}$
41	36725	36663	$76.12\ ^6I_{15/2} + 19.74\ ^6I_{13/2} + 2.59\ ^6I_{17/2}$
42		36689	$63.95\ ^6I_{13/2} + 34.61\ ^6I_{15/2} + 0.77\ ^6I_{17/2}$
43		36696	$64.41\ ^6I_{15/2} + 34.09\ ^6I_{13/2} + 0.74\ ^6I_{17/2}$
44		36701	$60.46\ ^6I_{13/2} + 38.14\ ^6I_{15/2} + 0.73\ ^6I_{17/2}$
45		36709	$62.26\ ^6I_{15/2} + 35.63\ ^6I_{13/2} + 1.18\ ^6I_{11/2}$
46		36714	$82.56\ ^6I_{15/2} + 15.83\ ^6I_{13/2} + 0.80\ ^6I_{17/2}$
47		36723	$71.72\ ^6I_{15/2} + 26.08\ ^6I_{13/2} + 1.27\ ^6I_{11/2}$
48		36731	$71.83\ ^6I_{15/2} + 26.57\ ^6I_{13/2} + 0.88\ ^6I_{17/2}$
49		36753	$52.22\ ^6I_{13/2} + 45.77\ ^6I_{15/2} + 1.16\ ^6I_{17/2}$
50		36756	$50.26\ ^6I_{13/2} + 47.79\ ^6I_{15/2} + 1.15\ ^6I_{11/2}$
51		36793	$61.83\ ^6I_{15/2} + 36.53\ ^6I_{13/2} + 1.02\ ^6I_{17/2}$
52		36793	$52.08\ ^6I_{15/2} + 46.12\ ^6I_{13/2} + 1.26\ ^6I_{17/2}$
53	$^6D_{9/2}$	39617	$99.01\ ^6D_{9/2} + 0.50\ ^6D_{7/2} + 0.18\ ^6D_{1/2}$
54	39779	39672	$98.50\ ^6D_{9/2} + 1.08\ ^6D_{7/2} + 0.12\ ^6D_{1/2}$
55		39776	$98.44\ ^6D_{9/2} + 1.31\ ^6D_{7/2} + 0.06\ ^6D_{5/2}$
56		39809	$99.39\ ^6D_{9/2} + 0.31\ ^6D_{7/2} + 0.07\ ^6P_{5/2}$
57		39947	$99.09\ ^6D_{9/2} + 0.43\ ^6D_{7/2} + 0.26\ ^6D_{1/2}$
58	$^6D_{1/2}$ 40621	40553	$73.98\ ^6D_{1/2} + 11.90\ ^6D_{7/2} + 8.71\ ^6D_{3/2}$
59	$^6D_{7/2}$	40661	$70.51\ ^6D_{7/2} + 22.33\ ^6D_{3/2} + 4.19\ ^6D_{1/2}$
60	40713	40691	$87.94\ ^6D_{7/2} + 5.82\ ^6D_{3/2} + 3.87\ ^6D_{5/2}$
61		40710	$94.21\ ^6D_{7/2} + 3.45\ ^6D_{5/2} + 1.14\ ^6D_{1/2}$
62		40719	$82.47\ ^6D_{7/2} + 9.30\ ^6D_{1/2} + 4.21\ ^6D_{5/2}$
63	$^6D_{3/2}$	40795	$63.05\ ^6D_{3/2} + 22.15\ ^6D_{7/2} + 13.44\ ^6D_{5/2}$
64	40851	40892	$58.96\ ^6D_{5/2} + 33.16\ ^6D_{3/2} + 6.37\ ^6D_{7/2}$
65	$^6D_{5/2}$	40955	$47.55\ ^6D_{5/2} + 36.75\ ^6D_{3/2} + 11.35\ ^6D_{7/2}$
66	40978	41028	$73.36\ ^6D_{5/2} + 17.28\ ^6D_{3/2} + 6.71\ ^6D_{7/2}$
67		41082	$87.80\ ^6D_{5/2} + 8.73\ ^6D_{3/2} + 2.17\ ^6D_{7/2}$

[a]Aqueous centroids (cm^{-1}).

42

Level	I. R.	$[(S,L)J]^{a}$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^7F_6$	0	$99.38\ ^7F_6 + 0.30\ ^7F_5 + 0.27\ ^7F_4$
2	Γ_1	74	1	$99.34\ ^7F_6 + 0.37\ ^7F_5 + 0.25\ ^7F_4$
3	Γ_2		119	$98.84\ ^7F_6 + 0.83\ ^7F_5 + 0.20\ ^7F_4$
4	Γ_2		124	$98.78\ ^7F_6 + 0.92\ ^7F_5 + 0.16\ ^7F_4$
5	Γ_1		340	$95.55\ ^7F_6 + 4.25\ ^7F_5 + 0.15\ ^7F_4$
6	Γ_1		362	$96.10\ ^7F_6 + 3.51\ ^7F_5 + 0.32\ ^7F_4$
7	Γ_2		481	$94.84\ ^7F_6 + 4.68\ ^7F_5 + 0.30\ ^7F_4$
8	Γ_2		557	$96.99\ ^7F_6 + 2.43\ ^7F_5 + 0.30\ ^7F_4$
9	Γ_1		604	$96.75\ ^7F_6 + 2.19\ ^7F_5 + 0.75\ ^7F_4$
10	Γ_1		768	$99.21\ ^7F_6 + 0.35\ ^7F_5 + 0.31\ ^7F_4$
11	Γ_2		770	$99.19\ ^7F_6 + 0.35\ ^7F_5 + 0.26\ ^7F_4$
12	Γ_1		841	$97.36\ ^7F_6 + 1.25\ ^7F_4 + 1.15\ ^7F_5$
13	Γ_2		841	$97.33\ ^7F_6 + 1.28\ ^7F_4 + 1.17\ ^7F_5$
14	Γ_2	$^7F_5$	2181	$97.81\ ^7F_5 + 0.92\ ^7F_4 + 0.75\ ^7F_6$
15	Γ_2	2112	2198	$97.71\ ^7F_5 + 0.96\ ^7F_4 + 0.82\ ^7F_6$
16	Γ_1		2355	$92.56\ ^7F_5 + 5.07\ ^7F_4 + 1.22\ ^7F_6$
17	Γ_1		2460	$91.22\ ^7F_5 + 5.29\ ^7F_4 + 2.66\ ^7F_6$
18	Γ_2		2507	$94.33\ ^7F_5 + 1.94\ ^7F_3 + 1.76\ ^7F_6$
19	Γ_1		2584	$91.93\ ^7F_5 + 4.50\ ^7F_6 + 2.28\ ^7F_4$
20	Γ_2		2617	$93.75\ ^7F_5 + 2.63\ ^7F_6 + 2.63\ ^7F_4$
21	Γ_2		2678	$91.44\ ^7F_5 + 3.84\ ^7F_6 + 3.54\ ^7F_4$
22	Γ_1		2696	$94.16\ ^7F_5 + 2.79\ ^7F_4 + 1.57\ ^7F_6$
23	Γ_1		2726	$94.74\ ^7F_5 + 2.06\ ^7F_6 + 1.79\ ^7F_4$
24	Γ_2		2735	$94.39\ ^7F_5 + 2.66\ ^7F_4 + 1.21\ ^7F_3$
25	Γ_2	$^7F_4$	3595	$90.69\ ^7F_4 + 3.75\ ^7F_3 + 3.38\ ^7F_5$
26	Γ_1	3370	3616	$93.49\ ^7F_4 + 3.05\ ^7F_5 + 1.14\ ^7F_3$
27	Γ_1		3641	$92.09\ ^7F_4 + 5.24\ ^7F_5 + 1.30\ ^7F_0$
28	Γ_1		3719	$94.35\ ^7F_4 + 2.56\ ^7F_5 + 1.67\ ^7F_2$
29	Γ_2		3726	$86.45\ ^7F_4 + 8.65\ ^7F_3 + 3.18\ ^7F_5$
30	Γ_2		3857	$87.56\ ^7F_4 + 5.63\ ^7F_3 + 5.31\ ^7F_5$
31	Γ_1		3869	$82.10\ ^7F_4 + 11.45\ ^7F_3 + 3.81\ ^7F_5$
32	Γ_1		4027	$86.42\ ^7F_4 + 8.24\ ^7F_3 + 2.53\ ^7F_5$
33	Γ_2		4029	$94.90\ ^7F_4 + 1.79\ ^7F_5 + 1.61\ ^7F_2$
34	Γ_2	$^7F_3$	4666	$87.52\ ^7F_3 + 7.88\ ^7F_1 + 3.97\ ^7F_4$
35	Γ_1	4344	4682	$75.22\ ^7F_3 + 10.30\ ^7F_2 + 9.27\ ^7F_4$
36	Γ_2		4708	$86.98\ ^7F_3 + 8.53\ ^7F_2 + 2.75\ ^7F_5$
37	Γ_1		4714	$85.77\ ^7F_3 + 5.43\ ^7F_4 + 4.11\ ^7F_1$
38	Γ_1		4826	$75.89\ ^7F_3 + 11.86\ ^7F_2 + 10.13\ ^7F_4$
39	Γ_2		4889	$74.05\ ^7F_3 + 16.14\ ^7F_2 + 8.95\ ^7F_4$
40	Γ_2		4981	$91.46\ ^7F_3 + 6.76\ ^7F_4 + 0.80\ ^7F_5$
41	Γ_2	$^7F_2$	5296	$71.96\ ^7F_2 + 24.73\ ^7F_3 + 2.15\ ^7F_4$
42	Γ_1	5028	5363	$79.11\ ^7F_2 + 9.33\ ^7F_0 + 7.73\ ^7F_3$
43	Γ_2	$^7F_1$	5559	$91.29\ ^7F_2 + 4.10\ ^7F_1 + 1.58\ ^7F_3$
44	Γ_1	5481	5707	$55.08\ ^7F_2 + 33.96\ ^7F_1 + 8.92\ ^7F_3$
45	Γ_1		5788	$46.71\ ^7F_2 + 39.60\ ^7F_1 + 12.64\ ^7F_3$
46	Γ_1		5826	$73.55\ ^7F_2 + 16.79\ ^7F_1 + 8.00\ ^7F_3$
47	Γ_2		6158	$90.88\ ^7F_1 + 3.98\ ^7F_3 + 3.66\ ^7F_2$
48	Γ_2		6189	$91.91\ ^7F_1 + 4.21\ ^7F_3 + 2.74\ ^7F_2$

Table 31. Predicted energy levels for Tb^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
49	Γ_1	$^7F_0$ 5703	6307	$85.53\ ^7F_0 + 12.33\ ^7F_2 + 1.90\ ^7F_4$
50	Γ_1	$^5D_4$	20834	$99.87\ ^5D_4 + 0.07\ ^5G_6 + 0.02\ ^5L_{10}$
51	Γ_1	20542	20836	$99.87\ ^5D_4 + 0.07\ ^5G_6 + 0.02\ ^5G_5$
52	Γ_2		20935	$99.73\ ^5D_4 + 0.16\ ^5G_6 + 0.04\ ^5G_5$
53	Γ_1		20939	$99.68\ ^5D_4 + 0.22\ ^5G_6 + 0.03\ ^5G_5$
54	Γ_2		20958	$99.82\ ^5D_4 + 0.06\ ^5G_6 + 0.06\ ^5D_3$
55	Γ_2		20970	$99.85\ ^5D_4 + 0.05\ ^5G_6 + 0.05\ ^5D_3$
56	Γ_1		21025	$99.83\ ^5D_4 + 0.08\ ^5G_6 + 0.04\ ^5D_3$
57	Γ_1		21074	$99.88\ ^5D_4 + 0.03\ ^5G_6 + 0.02\ ^5L_{10}$
58	Γ_2		21078	$99.88\ ^5D_4 + 0.05\ ^5G_6 + 0.02\ ^5L_{10}$
59	Γ_1	$^5G_6$	26498	$94.72\ ^5G_6 + 2.60\ ^5D_3 + 1.27\ ^5L_{10}$
60	Γ_1	26424	26500	$94.74\ ^5G_6 + 2.60\ ^5D_3 + 1.31\ ^5L_{10}$
61	Γ_2	$^5D_3$	26580	$69.67\ ^5G_6 + 29.04\ ^5D_3 + 0.49\ ^5L_{10}$
62	Γ_2	26336	26601	$74.49\ ^5G_6 + 23.56\ ^5D_3 + 0.95\ ^5L_{10}$
63	Γ_1		26688	$61.68\ ^5D_3 + 36.35\ ^5G_6 + 0.83\ ^5G_5$
64	Γ_1		26724	$81.15\ ^5D_3 + 17.78\ ^5G_6 + 0.34\ ^5G_5$
65	Γ_1		26731	$49.31\ ^5G_6 + 45.29\ ^5D_3 + 3.62\ ^5L_{10}$
66	Γ_2		26737	$82.48\ ^5D_3 + 14.96\ ^5G_6 + 1.18\ ^5G_5$
67	Γ_2		26743	$68.35\ ^5D_3 + 29.51\ ^5G_6 + 1.17\ ^5L_{10}$
68	Γ_1		26756	$62.83\ ^5D_3 + 34.10\ ^5G_6 + 1.99\ ^5L_{10}$
69	Γ_2		26769	$83.39\ ^5D_3 + 15.23\ ^5G_6 + 0.73\ ^5G_5$
70	Γ_2		26777	$72.33\ ^5D_3 + 26.22\ ^5G_6 + 0.93\ ^5L_{10}$
71	Γ_1		26794	$76.58\ ^5G_6 + 21.27\ ^5D_3 + 1.00\ ^5L_{10}$
72	Γ_2		26842	$77.59\ ^5G_6 + 14.07\ ^5D_3 + 6.02\ ^5L_{10}$
73	Γ_2		26931	$85.79\ ^5G_6 + 10.78\ ^5D_3 + 1.37\ ^5G_5$
74	Γ_1		27003	$73.95\ ^5G_6 + 13.32\ ^5L_{10} + 10.29\ ^5D_3$
75	Γ_1		27012	$93.57\ ^5G_6 + 2.87\ ^5D_3 + 2.16\ ^5L_{10}$
76	Γ_2		27020	$87.78\ ^5G_6 + 7.46\ ^5L_{10} + 2.67\ ^5D_3$
77	Γ_1		27056	$88.18\ ^5G_6 + 5.09\ ^5D_3 + 4.67\ ^5L_{10}$
78	Γ_2		27090	$83.53\ ^5G_6 + 8.40\ ^5D_3 + 5.89\ ^5L_{10}$
79	Γ_2	$^5L_{10}$	27142	$81.76\ ^5L_{10} + 17.33\ ^5G_6 + 0.45\ ^5D_3$
80	Γ_1	27146	27145	$79.73\ ^5L_{10} + 19.04\ ^5G_6 + 0.67\ ^5D_3$
81	Γ_1	$^5G_5$	27224	$98.05\ ^5L_{10} + 1.39\ ^5G_6 + 0.45\ ^5L_9$
82	Γ_1	27795	27225	$97.67\ ^5L_{10} + 1.69\ ^5G_6 + 0.51\ ^5L_9$
83	Γ_2		27294	$98.73\ ^5L_{10} + 0.56\ ^5G_6 + 0.43\ ^5L_9$
84	Γ_2		27299	$98.21\ ^5L_{10} + 0.93\ ^5G_6 + 0.56\ ^5L_9$
85	Γ_1		27449	$97.06\ ^5L_{10} + 1.60\ ^5L_9 + 1.17\ ^5G_6$
86	Γ_1		27476	$96.13\ ^5L_{10} + 2.27\ ^5L_9 + 1.41\ ^5G_6$
87	Γ_2		27477	$93.69\ ^5L_{10} + 4.30\ ^5L_9 + 1.72\ ^5G_6$
88	Γ_1		27491	$95.83\ ^5L_{10} + 2.98\ ^5L_9 + 1.09\ ^5G_6$
89	Γ_2		27544	$97.24\ ^5L_{10} + 1.38\ ^5L_9 + 0.87\ ^5G_6$
90	Γ_2		27600	$96.09\ ^5L_{10} + 1.87\ ^5G_6 + 1.38\ ^5L_9$
91	Γ_1		27646	$97.19\ ^5L_{10} + 1.35\ ^5L_9 + 1.35\ ^5G_6$
92	Γ_1		27690	$97.46\ ^5L_{10} + 1.71\ ^5L_9 + 0.68\ ^5G_6$
93	Γ_2		27690	$97.55\ ^5L_{10} + 1.64\ ^5L_9 + 0.44\ ^5G_6$
94	Γ_2		27771	$96.58\ ^5L_{10} + 1.76\ ^5G_5 + 0.84\ ^5G_6$
95	Γ_1		27773	$96.97\ ^5L_{10} + 1.12\ ^5G_6 + 1.09\ ^5G_5$
96	Γ_2		27932	$48.91\ ^5G_5 + 48.17\ ^5L_{10} + 1.50\ ^5G_4$

Table 31 (cont'd). Predicted energy levels for Tb^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	I. R.	[(S,L)J][a]	Energy (cm^{-1})	Free ion mixture (%)
97	Γ$_2$		27939	53.31 $^5L_{10}$ + 44.33 $^5G_5$ + 1.21 $^5G_4$
98	Γ$_1$		27977	90.21 $^5L_{10}$ + 8.83 $^5G_5$ + 0.51 $^5L_9$
99	Γ$_1$		27981	89.45 $^5L_{10}$ + 9.64 $^5G_5$ + 0.46 $^5L_9$
100	Γ$_2$		28036	50.38 $^5L_{10}$ + 44.99 $^5G_5$ + 2.55 $^5G_4$
101	Γ$_2$		28039	51.89 $^5G_5$ + 43.56 $^5L_{10}$ + 2.94 $^5G_4$
102	Γ$_1$		28145	84.92 $^5G_5$ + 8.04 $^5L_{10}$ + 3.92 $^5G_4$
103	Γ$_1$		28161	86.76 $^5G_5$ + 8.61 $^5L_{10}$ + 2.84 $^5D_2$
104	Γ$_2$		28182	84.13 $^5G_5$ + 8.74 $^5G_4$ + 3.07 $^5L_{10}$
105	Γ$_1$		28255	87.10 $^5G_5$ + 9.53 $^5G_4$ + 1.30 $^5L_{10}$
106	Γ$_2$		28259	94.20 $^5G_5$ + 1.99 $^5G_4$ + 1.64 $^5G_6$
107	Γ$_1$		28282	85.85 $^5G_5$ + 9.41 $^5G_4$ + 1.81 $^5D_2$
108	Γ$_2$		28349	87.48 $^5G_5$ + 5.69 $^5G_4$ + 4.70 $^5D_2$
109	Γ$_2$		28366	90.89 $^5G_5$ + 4.61 $^5D_2$ + 2.09 $^5G_4$
110	Γ$_1$		28377	83.71 $^5G_5$ + 9.34 $^5G_4$ + 4.12 $^5D_2$
111	Γ$_2$	$^5D_2$	28490	85.95 $^5D_2$ + 8.57 $^5G_5$ + 4.48 $^5G_4$
112	Γ$_1$	28150	28505	82.53 $^5D_2$ + 13.15 $^5G_4$ + 3.61 $^5G_5$
113	Γ$_2$	$^5G_4$	28562	73.91 $^5D_2$ + 18.43 $^5G_4$ + 5.90 $^5G_5$
114	Γ$_1$	28307	28595	52.44 $^5G_4$ + 43.56 $^5D_2$ + 2.03 $^5L_9$
115	Γ$_1$	$^5L_9$	28624	84.77 $^5G_4$ + 7.18 $^5D_2$ + 4.39 $^5G_5$
116	Γ$_2$	28503	28640	96.68 $^5L_9$ + 2.05 $^5G_4$ + 0.65 $^5L_{10}$
117	Γ$_2$		28642	96.27 $^5L_9$ + 2.17 $^5G_4$ + 0.62 $^5L_{10}$
118	Γ$_1$		28657	71.65 $^5D_2$ + 18.79 $^5G_4$ + 5.54 $^5L_9$
119	Γ$_1$		28668	35.09 $^5L_9$ + 31.45 $^5G_4$ + 22.96 $^5D_2$
120	Γ$_2$		28677	92.70 $^5L_9$ + 3.58 $^5L_{10}$ + 1.33 $^5G_5$
121	Γ$_1$		28681	56.52 $^5L_9$ + 20.48 $^5D_2$ + 13.89 $^5G_4$
122	Γ$_1$		28751	92.33 $^5L_9$ + 3.56 $^5G_4$ + 2.37 $^5D_2$
123	Γ$_1$		28761	89.88 $^5L_9$ + 6.91 $^5G_4$ + 1.30 $^5L_{10}$
124	Γ$_2$		28765	90.06 $^5G_4$ + 4.95 $^5G_5$ + 4.56 $^5L_9$
125	Γ$_2$		28797	86.05 $^5G_4$ + 5.17 $^5G_5$ + 4.30 $^5L_9$
126	Γ$_1$		28853	80.07 $^5G_4$ + 11.03 $^5D_2$ + 6.59 $^5L_9$
127	Γ$_2$		28860	60.88 $^5G_4$ + 24.35 $^5L_9$ + 7.02 $^5D_2$
128	Γ$_1$		28875	75.75 $^5G_4$ + 13.01 $^5D_2$ + 5.53 $^5G_5$
129	Γ$_2$		28879	49.16 $^5G_4$ + 35.59 $^5L_9$ + 8.61 $^5D_2$
130	Γ$_1$		28881	66.18 $^5G_4$ + 15.63 $^5L_9$ + 9.85 $^5D_2$
131	Γ$_2$		28911	61.97 $^5L_9$ + 35.02 $^5G_4$ + 1.73 $^5D_2$
132	Γ$_2$		28924	81.13 $^5L_9$ + 14.83 $^5G_4$ + 1.58 $^5D_2$
133	Γ$_1$		28966	85.16 $^5L_9$ + 11.49 $^5G_4$ + 1.22 $^5D_2$
134	Γ$_2$		28974	95.37 $^5L_9$ + 2.71 $^5G_4$ + 1.41 $^5L_{10}$
135	Γ$_1$		28991	97.92 $^5L_9$ + 0.90 $^5G_4$ + 0.77 $^5L_{10}$
136	Γ$_1$		29041	98.17 $^5L_9$ + 0.71 $^5L_{10}$ + 0.65 $^5G_6$
137	Γ$_2$		29068	98.60 $^5L_9$ + 0.81 $^5G_6$ + 0.32 $^5L_{10}$
138	Γ$_2$		29141	96.15 $^5L_9$ + 2.51 $^5G_4$ + 0.75 $^5G_6$
139	Γ$_1$		29151	95.69 $^5L_9$ + 2.98 $^5G_4$ + 0.90 $^5G_6$
140	Γ$_1$		29249	96.68 $^5L_9$ + 2.04 $^5L_{10}$ + 0.99 $^5G_4$
141	Γ$_2$		29249	96.97 $^5L_9$ + 1.93 $^5L_{10}$ + 0.76 $^5G_4$
142	Γ$_1$		29255	96.79 $^5L_9$ + 1.85 $^5L_{10}$ + 0.92 $^5G_4$
143	Γ$_2$		29257	96.77 $^5L_9$ + 1.68 $^5L_{10}$ + 1.06 $^5G_4$

[a] Aqueous centroids (cm^{-1}).

Table 32. Predicted energy levels for Dy³⁺ in Ca₅(PO₄)₃F, C_s site. B_{nm} from table 9.

Level	$[(S,L)J]^a$	Energy (cm⁻¹)	Free ion mixture (%)
1	$^6H_{15/2}$	0	$99.72\,^6H_{15/2} + 0.12\,^6F_{11/2} + 0.11\,^6H_{13/2}$
2	40	286	$99.29\,^6H_{15/2} + 0.60\,^6H_{13/2} + 0.07\,^6F_{9/2}$
3		461	$99.37\,^6H_{15/2} + 0.31\,^6F_{11/2} + 0.26\,^6H_{13/2}$
4		564	$99.32\,^6H_{15/2} + 0.49\,^6H_{13/2} + 0.10\,^6F_{11/2}$
5		722	$99.49\,^6H_{15/2} + 0.37\,^6H_{13/2} + 0.06\,^6F_{11/2}$
6		765	$99.36\,^6H_{15/2} + 0.44\,^6H_{13/2} + 0.11\,^6F_{11/2}$
7		883	$99.38\,^6H_{15/2} + 0.28\,^6F_{11/2} + 0.21\,^6H_{13/2}$
8		1016	$99.56\,^6H_{15/2} + 0.23\,^6F_{11/2} + 0.10\,^6F_{9/2}$
9	$^6H_{13/2}$	3672	$98.71\,^6H_{13/2} + 0.58\,^6H_{15/2} + 0.34\,^6H_{11/2}$
10	3506	3869	$97.43\,^6H_{13/2} + 1.48\,^6H_{11/2} + 0.73\,^6H_{15/2}$
11		4029	$98.20\,^6H_{13/2} + 1.04\,^6H_{11/2} + 0.40\,^6H_{15/2}$
12		4090	$98.75\,^6H_{13/2} + 0.40\,^6H_{11/2} + 0.28\,^6H_{15/2}$
13		4123	$97.96\,^6H_{13/2} + 1.00\,^6H_{11/2} + 0.42\,^6F_{11/2}$
14		4194	$98.11\,^6H_{13/2} + 0.94\,^6H_{11/2} + 0.25\,^6H_{15/2}$
15		4361	$98.76\,^6H_{13/2} + 0.38\,^6H_{11/2} + 0.25\,^6F_{11/2}$
16	$^6H_{11/2}$	6117	$97.22\,^6H_{11/2} + 1.63\,^6H_{13/2} + 0.45\,^6H_{9/2}$
17	5833	6217	$95.86\,^6H_{11/2} + 1.61\,^6H_{9/2} + 1.50\,^6H_{13/2}$
18		6337	$96.90\,^6H_{11/2} + 0.86\,^6H_{9/2} + 0.76\,^6F_{9/2}$
19		6436	$96.19\,^6H_{11/2} + 1.52\,^6H_{9/2} + 0.80\,^6F_{9/2}$
20		6534	$96.72\,^6H_{11/2} + 1.07\,^6H_{9/2} + 0.87\,^6F_{11/2}$
21		6610	$97.52\,^6H_{11/2} + 0.90\,^6F_{11/2} + 0.85\,^6H_{13/2}$
22	$^6H_{9/2}$	7980	$81.83\,^6H_{9/2} + 13.74\,^6F_{11/2} + 2.46\,^6H_{11/2}$
23	7692	8027	$69.92\,^6H_{9/2} + 24.75\,^6F_{11/2} + 2.61\,^6H_{7/2}$
24	$^6F_{11/2}$	8128	$55.99\,^6F_{11/2} + 40.68\,^6H_{9/2} + 0.87\,^6H_{7/2}$
25	7730	8196	$60.12\,^6F_{11/2} + 37.36\,^6H_{9/2} + 0.87\,^6F_{9/2}$
26		8250	$61.22\,^6F_{11/2} + 35.67\,^6H_{9/2} + 1.10\,^6F_{9/2}$
27		8273	$49.07\,^6F_{11/2} + 47.09\,^6H_{9/2} + 1.04\,^6H_{7/2}$
28		8321	$59.06\,^6F_{11/2} + 38.73\,^6H_{9/2} + 0.61\,^6F_{9/2}$
29		8366	$54.64\,^6F_{11/2} + 42.78\,^6H_{9/2} + 1.18\,^6F_{9/2}$
30		8424	$64.59\,^6F_{11/2} + 33.38\,^6H_{9/2} + 0.58\,^6H_{7/2}$
31		8541	$84.55\,^6F_{11/2} + 12.91\,^6H_{9/2} + 0.93\,^6H_{11/2}$
32		8625	$63.34\,^6F_{11/2} + 33.26\,^6H_{9/2} + 1.31\,^6H_{7/2}$
33	$^6H_{7/2}$	9401	$62.72\,^6H_{7/2} + 30.69\,^6F_{9/2} + 4.43\,^6H_{9/2}$
34	9115	9469	$73.28\,^6H_{7/2} + 18.69\,^6F_{9/2} + 4.98\,^6H_{5/2}$
35	$^6F_{9/2}$	9606	$59.63\,^6F_{9/2} + 37.47\,^6H_{7/2} + 0.87\,^6H_{9/2}$
36	9087	9650	$55.16\,^6F_{9/2} + 40.01\,^6H_{7/2} + 1.42\,^6H_{9/2}$
37		9689	$82.18\,^6F_{9/2} + 14.41\,^6H_{7/2} + 1.34\,^6H_{9/2}$
38		9741	$88.19\,^6F_{9/2} + 9.44\,^6H_{7/2} + 0.90\,^6H_{9/2}$
39		9819	$66.88\,^6F_{9/2} + 27.38\,^6H_{7/2} + 2.60\,^6H_{5/2}$
40		9833	$50.40\,^6F_{9/2} + 42.72\,^6H_{7/2} + 3.61\,^6H_{5/2}$
41		9964	$59.75\,^6H_{7/2} + 31.76\,^6F_{9/2} + 3.74\,^6H_{5/2}$
42	$^6H_{5/2}$	10546	$83.63\,^6H_{5/2} + 11.77\,^6H_{7/2} + 2.11\,^6F_{9/2}$
43	10169	10764	$91.74\,^6H_{5/2} + 2.73\,^6H_{7/2} + 2.23\,^6F_{7/2}$
44		10947	$87.71\,^6H_{5/2} + 8.61\,^6F_{7/2} + 1.10\,^6H_{7/2}$
45	$^6F_{7/2}$	11621	$95.78\,^6F_{7/2} + 2.41\,^6H_{5/2} + 0.67\,^6H_{7/2}$
46	11025	11649	$92.59\,^6F_{7/2} + 4.84\,^6H_{5/2} + 1.14\,^6H_{7/2}$
47		11694	$97.66\,^6F_{7/2} + 0.85\,^6H_{7/2} + 0.48\,^6H_{9/2}$
48		11736	$93.35\,^6F_{7/2} + 3.90\,^6H_{5/2} + 1.38\,^6H_{7/2}$

Table 32 (cont'd). Predicted energy levels for Dy^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_s$ site. B$_{nm}$ from table 9.

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
49	$^6F_{5/2}$	13008	$96.41\ ^6F_{5/2} + 1.23\ ^6H_{5/2} + 1.04\ ^6F_{3/2}$
50	12432	13052	$97.37\ ^6F_{5/2} + 1.06\ ^6F_{3/2} + 0.67\ ^6H_{7/2}$
51		13122	$97.58\ ^6F_{5/2} + 1.24\ ^6H_{5/2} + 0.38\ ^6F_{7/2}$
52	$^6F_{3/2}$	13825	$96.61\ ^6F_{3/2} + 1.79\ ^6F_{1/2} + 0.58\ ^6H_{5/2}$
53	13212	13865	$96.27\ ^6F_{3/2} + 2.11\ ^6F_{5/2} + 0.69\ ^6H_{5/2}$
54	$^6F_{1/2}$ 13760	14401	$96.62\ ^6F_{1/2} + 2.01\ ^6F_{3/2} + 0.54\ ^6H_{5/2}$
55	$^4F_{9/2}$	21456	$97.42\ ^4F_{9/2} + 2.02\ ^4I_{15/2} + 0.55\ ^4G_{11/2}$
56	21144	21560	$96.33\ ^4F_{9/2} + 2.68\ ^4I_{15/2} + 0.99\ ^4G_{11/2}$
57		21633	$97.24\ ^4F_{9/2} + 1.73\ ^4I_{15/2} + 1.03\ ^4G_{11/2}$
58		21774	$92.89\ ^4F_{9/2} + 5.53\ ^4I_{15/2} + 1.57\ ^4G_{11/2}$
59		21865	$93.57\ ^4F_{9/2} + 5.38\ ^4I_{15/2} + 1.05\ ^4G_{11/2}$
60	$^4I_{15/2}$	22457	$98.87\ ^4I_{15/2} + 0.94\ ^4G_{11/2} + 0.19\ ^4F_{9/2}$
61	22293	22708	$93.35\ ^4I_{15/2} + 6.10\ ^4F_{9/2} + 0.55\ ^4G_{11/2}$
62		22746	$97.43\ ^4I_{15/2} + 1.66\ ^4G_{11/2} + 0.90\ ^4F_{9/2}$
63		22889	$95.14\ ^4I_{15/2} + 3.39\ ^4F_{9/2} + 1.46\ ^4G_{11/2}$
64		22957	$96.06\ ^4I_{15/2} + 3.08\ ^4G_{11/2} + 0.86\ ^4F_{9/2}$
65		23003	$96.88\ ^4I_{15/2} + 2.06\ ^4G_{11/2} + 1.05\ ^4F_{9/2}$
66		23045	$94.90\ ^4I_{15/2} + 2.57\ ^4F_{9/2} + 2.53\ ^4G_{11/2}$
67		23219	$95.57\ ^4I_{15/2} + 2.30\ ^4G_{11/2} + 2.13\ ^4F_{9/2}$
68	$^4G_{11/2}$	23669	$96.58\ ^4G_{11/2} + 3.17\ ^4I_{15/2} + 0.25\ ^4F_{9/2}$
69	23321	23788	$95.24\ ^4G_{11/2} + 3.76\ ^4I_{15/2} + 1.00\ ^4F_{9/2}$
70		23944	$95.57\ ^4G_{11/2} + 2.58\ ^4I_{15/2} + 1.85\ ^4F_{9/2}$
71		24034	$97.08\ ^4G_{11/2} + 1.57\ ^4I_{15/2} + 1.35\ ^4F_{9/2}$
72		24088	$97.85\ ^4G_{11/2} + 1.58\ ^4I_{15/2} + 0.56\ ^4F_{9/2}$
73		24120	$97.90\ ^4G_{11/2} + 1.78\ ^4I_{15/2} + 0.32\ ^4F_{9/2}$

^{a}Aqueous centroids (cm^{-1}).

Table 33. Predicted energy levels for Ho^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_s$ site. B$_{nm}$ from table 9.

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^5I_8$	0	$99.93\ ^5I_8 + 0.04\ ^5I_7 + 0.01\ ^5G_6$
2	Γ_1	80	2	$99.93\ ^5I_8 + 0.04\ ^5I_7 + 0.01\ ^5G_6$
3	Γ_2		94	$99.89\ ^5I_8 + 0.06\ ^5I_7 + 0.02\ ^5F_5$
4	Γ_2		105	$99.89\ ^5I_8 + 0.07\ ^5I_7 + 0.02\ ^5F_5$
5	Γ_1		163	$99.91\ ^5I_8 + 0.05\ ^5I_7 + 0.02\ ^5G_6$
6	Γ_2		178	$99.93\ ^5I_8 + 0.03\ ^5I_7 + 0.02\ ^5G_6$
7	Γ_1		238	$99.82\ ^5I_8 + 0.13\ ^5I_7 + 0.02\ ^5F_5$
8	Γ_1		290	$99.91\ ^5I_8 + 0.06\ ^5I_7 + 0.01\ ^5G_6$
9	Γ_2		316	$99.90\ ^5I_8 + 0.04\ ^5I_7 + 0.03\ ^5G_6$
10	Γ_1		343	$99.93\ ^5I_8 + 0.03\ ^5I_7 + 0.02\ ^5G_6$
11	Γ_2		395	$99.89\ ^5I_8 + 0.06\ ^5I_7 + 0.03\ ^5G_6$
12	Γ_2		403	$99.90\ ^5I_8 + 0.05\ ^5I_7 + 0.04\ ^5G_6$
13	Γ_1		413	$99.89\ ^5I_8 + 0.05\ ^5I_7 + 0.04\ ^5G_6$
14	Γ_2		428	$99.85\ ^5I_8 + 0.11\ ^5I_7 + 0.02\ ^5G_6$
15	Γ_1		467	$99.88\ ^5I_8 + 0.06\ ^5I_7 + 0.04\ ^5G_6$
16	Γ_1		553	$99.85\ ^5I_8 + 0.06\ ^5I_7 + 0.04\ ^5G_6$
17	Γ_2		556	$99.86\ ^5I_8 + 0.06\ ^5I_7 + 0.05\ ^5G_6$

Table 33 (cont'd). Predicted energy levels for Ho^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	I. R.	[(S,L)J][a]	Energy (cm^{-1})	Free ion mixture (%)
18	Γ_2	$^5I_7$	5116	99.81 $^5I_7$ + 0.08 $^5I_6$ + 0.05 $^5I_8$
19	Γ_1	5116	5116	99.81 $^5I_7$ + 0.08 $^5I_6$ + 0.06 $^5I_8$
20	Γ_2		5229	99.72 $^5I_7$ + 0.13 $^5I_6$ + 0.10 $^5I_8$
21	Γ_1		5230	99.68 $^5I_7$ + 0.13 $^5I_8$ + 0.13 $^5I_6$
22	Γ_2		5282	99.84 $^5I_7$ + 0.06 $^5I_8$ + 0.05 $^5I_6$
23	Γ_1		5283	99.84 $^5I_7$ + 0.07 $^5I_8$ + 0.03 $^5I_6$
24	Γ_2		5332	99.68 $^5I_7$ + 0.17 $^5I_6$ + 0.09 $^5I_8$
25	Γ_2		5335	99.64 $^5I_7$ + 0.16 $^5I_6$ + 0.11 $^5I_8$
26	Γ_1		5392	99.69 $^5I_7$ + 0.20 $^5I_6$ + 0.04 $^5I_8$
27	Γ_2		5398	99.79 $^5I_7$ + 0.11 $^5I_6$ + 0.04 $^5I_8$
28	Γ_1		5403	99.68 $^5I_7$ + 0.18 $^5I_6$ + 0.06 $^5I_8$
29	Γ_1		5407	99.85 $^5I_7$ + 0.05 $^5I_8$ + 0.03 $^5F_5$
30	Γ_2		5424	99.77 $^5I_7$ + 0.11 $^5I_6$ + 0.04 $^5F_5$
31	Γ_1		5496	99.68 $^5I_7$ + 0.14 $^5I_6$ + 0.06 $^5I_8$
32	Γ_2		5497	99.73 $^5I_7$ + 0.11 $^5I_6$ + 0.05 $^5I_8$
33	Γ_1	$^5I_6$	8635	99.62 $^5I_6$ + 0.14 $^5I_7$ + 0.14 $^5I_5$
34	Γ_1	8614	8635	99.59 $^5I_6$ + 0.16 $^5I_7$ + 0.15 $^5I_5$
35	Γ_2		8753	99.36 $^5I_6$ + 0.29 $^5I_7$ + 0.25 $^5I_5$
36	Γ_2		8760	99.34 $^5I_6$ + 0.32 $^5I_5$ + 0.23 $^5I_7$
37	Γ_1		8806	99.72 $^5I_6$ + 0.12 $^5I_7$ + 0.07 $^5I_5$
38	Γ_2		8813	99.68 $^5I_6$ + 0.17 $^5I_5$ + 0.09 $^5I_7$
39	Γ_1		8847	99.36 $^5I_6$ + 0.36 $^5I_5$ + 0.16 $^5I_7$
40	Γ_1		8854	99.43 $^5I_6$ + 0.35 $^5I_5$ + 0.10 $^5I_7$
41	Γ_2		8881	99.47 $^5I_6$ + 0.38 $^5I_5$ + 0.04 $^5F_5$
42	Γ_1		8916	99.47 $^5I_6$ + 0.40 $^5I_5$ + 0.04 $^5I_7$
43	Γ_2		8919	99.62 $^5I_6$ + 0.21 $^5I_5$ + 0.05 $^5I_7$
44	Γ_2		8966	99.31 $^5I_6$ + 0.40 $^5I_5$ + 0.15 $^5I_7$
45	Γ_1		8972	99.52 $^5I_6$ + 0.21 $^5I_5$ + 0.13 $^5I_7$
46	Γ_2	$^5I_5$	11211	99.03 $^5I_5$ + 0.46 $^5I_6$ + 0.37 $^5I_4$
47	Γ_2	11164	11216	99.31 $^5I_5$ + 0.38 $^5I_6$ + 0.18 $^5I_4$
48	Γ_1		11342	98.81 $^5I_5$ + 0.55 $^5I_6$ + 0.53 $^5I_4$
49	Γ_1		11349	98.97 $^5I_5$ + 0.53 $^5I_6$ + 0.44 $^5I_4$
50	Γ_1		11375	99.20 $^5I_5$ + 0.42 $^5I_4$ + 0.31 $^5I_6$
51	Γ_2		11382	99.47 $^5I_5$ + 0.30 $^5I_6$ + 0.16 $^5I_4$
52	Γ_2		11414	99.34 $^5I_5$ + 0.45 $^5I_4$ + 0.10 $^5I_6$
53	Γ_2		11438	99.33 $^5I_5$ + 0.38 $^5I_4$ + 0.16 $^5I_6$
54	Γ_1		11454	99.15 $^5I_5$ + 0.67 $^5I_4$ + 0.06 $^5I_6$
55	Γ_1		11504	99.00 $^5I_5$ + 0.63 $^5I_4$ + 0.25 $^5I_6$
56	Γ_2		11506	98.84 $^5I_5$ + 0.71 $^5I_4$ + 0.33 $^5I_6$
57	Γ_1	$^5I_4$	13205	99.21 $^5I_4$ + 0.63 $^5I_5$ + 0.06 $^5I_6$
58	Γ_1	13219	13241	98.58 $^5I_4$ + 1.29 $^5I_5$ + 0.03 $^5F_2$
59	Γ_2		13360	99.47 $^5I_4$ + 0.39 $^5I_5$ + 0.04 $^5F_3$
60	Γ_1		13425	99.47 $^5I_4$ + 0.38 $^5I_5$ + 0.06 $^5I_6$
61	Γ_2		13431	99.09 $^5I_4$ + 0.71 $^5I_5$ + 0.08 $^5F_2$
62	Γ_2		13504	99.17 $^5I_4$ + 0.69 $^5I_5$ + 0.05 $^5I_6$
63	Γ_1		13527	99.72 $^5I_4$ + 0.13 $^5I_5$ + 0.03 $^5I_6$
64	Γ_2		13655	99.37 $^5I_4$ + 0.49 $^5I_5$ + 0.03 $^5F_1$
65	Γ_1		13679	99.58 $^5I_4$ + 0.27 $^5I_5$ + 0.05 $^5I_6$

	Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
Table 33 (cont'd). Predicted energy levels for Ho^{3+} in Ca$_5$(PO$_4$)$_3$F, C$_s$ site. B$_{nm}$ from table 9.	66	Γ_1	$^5F_5$	15552	99.51 $^5F_5$ + 0.19 $^5F_4$ + 0.11 $^5G_6$
	67	Γ_2	15519	15555	99.54 $^5F_5$ + 0.14 $^5F_4$ + 0.10 $^5G_6$
	68	Γ_2		15608	99.34 $^5F_5$ + 0.32 $^5G_6$ + 0.16 $^5F_4$
	69	Γ_1		15634	99.51 $^5F_5$ + 0.28 $^5G_6$ + 0.06 $^5F_4$
	70	Γ_2		15637	99.05 $^5F_5$ + 0.38 $^5G_6$ + 0.36 $^5F_4$
	71	Γ_1		15667	99.17 $^5F_5$ + 0.40 $^5G_6$ + 0.26 $^5F_4$
	72	Γ_2		15716	99.18 $^5F_5$ + 0.44 $^5F_4$ + 0.18 $^5G_6$
	73	Γ_1		15863	99.37 $^5F_5$ + 0.24 $^5F_4$ + 0.20 $^5G_6$
	74	Γ_1		15874	99.36 $^5F_5$ + 0.29 $^5F_4$ + 0.18 $^5G_6$
	75	Γ_2		15910	99.49 $^5F_5$ + 0.27 $^5G_6$ + 0.05 $^3G_5$
	76	Γ_2		15918	99.50 $^5F_5$ + 0.24 $^5G_6$ + 0.05 $^3G_5$
	77	Γ_2	$^5S_2$	18527	95.89 $^5S_2$ + 3.45 $^5F_4$ + 0.51 $^5G_6$
	78	Γ_1	18353	18540	87.19 $^5S_2$+12.48 $^5F_4$ + 0.17 $^5G_6$
	79	Γ_1		18558	97.94 $^5S_2$ + 1.56 $^5F_4$ + 0.28 $^5G_6$
	80	Γ_2		18564	94.07 $^5S_2$ + 5.49 $^5F_4$ + 0.19 $^5G_6$
	81	Γ_1		18568	96.66 $^5S_2$ + 2.64 $^5F_4$ + 0.61 $^5G_6$
	82	Γ_2	$^5F_4$	18705	95.74 $^5F_4$ + 3.33 $^5S_2$ + 0.35 $^5F_3$
	83	Γ_1	18612	18732	87.29 $^5F_4$+11.75 $^5S_2$ + 0.34 $^5F_2$
	84	Γ_1		18750	95.91 $^5F_4$ + 2.95 $^5S_2$ + 0.34 $^5G_6$
	85	Γ_2		18784	96.11 $^5F_4$ + 3.02 $^5S_2$ + 0.23 $^5F_2$
	86	Γ_1		18831	98.44 $^5F_4$ + 0.55 $^5G_6$ + 0.41 $^5F_3$
	87	Γ_2		18838	95.71 $^5F_4$ + 2.53 $^5S_2$ + 0.60 $^5G_6$
	88	Γ_2		18874	98.35 $^5F_4$ + 0.54 $^5G_6$ + 0.48 $^5F_5$
	89	Γ_1		18967	97.91 $^5F_4$ + 0.96 $^5S_2$ + 0.25 $^5F_3$
	90	Γ_1		18973	97.84 $^5F_4$ + 1.05 $^5S_2$ + 0.28 $^5F_3$
	91	Γ_2	$^3F_3$	20706	98.57 $^5F_3$ + 0.51 $^5F_2$ + 0.28 $^3G_5$
	92	Γ_1	20672	20786	96.24 $^5F_3$ + 1.90 $^5F_2$ + 0.52 $^5F_1$
	93	Γ_1		20821	95.22 $^5F_3$ + 2.77 $^5F_2$ + 0.81 $^5G_6$
	94	Γ_1		20897	93.99 $^5F_3$ + 4.31 $^5F_2$ + 0.68 $^5G_6$
	95	Γ_2		20899	92.78 $^5F_3$ + 5.42 $^5F_2$ + 0.77 $^5G_6$
	96	Γ_2		21007	93.86 $^5F_3$ + 4.53 $^5F_2$ + 0.63 $^5G_6$
	97	Γ_2		21025	96.75 $^5F_3$ + 1.64 $^5F_2$ + 0.47 $^5G_6$
	98	Γ_2	$^5F_2$	21253	89.00 $^5F_2$ + 9.37 $^5F_3$ + 1.03 $^5F_1$
	99	Γ_1	21130	21327	98.47 $^5F_2$ + 0.39 $^3K_8$ + 0.38 $^5F_4$
	100	Γ_1	$^3K_8$	21381	92.21 $^5F_2$ + 5.35 $^5F_3$ + 1.13 $^3K_8$
	101	Γ_2	21307	21382	93.79 $^5F_2$ + 2.65 $^5F_3$ + 1.14 $^5F_1$
	102	Γ_2		21427	99.62 $^3K_8$ + 0.21 $^5G_6$ + 0.11 $^5F_2$
	103	Γ_1		21428	99.23 $^3K_8$ + 0.49 $^5F_2$ + 0.22 $^5G_6$
	104	Γ_1		21461	99.20 $^3K_8$ + 0.68 $^5F_2$ + 0.06 $^5G_6$
	105	Γ_1		21478	86.72 $^3K_8$+12.44 $^5F_2$ + 0.50 $^5F_3$
	106	Γ_2		21479	99.12 $^3K_8$ + 0.69 $^5F_2$ + 0.10 $^5G_6$
	107	Γ_2		21483	99.88 $^3K_8$ + 0.07 $^5G_6$ + 0.03 $^5F_2$
	108	Γ_2		21485	99.68 $^3K_8$ + 0.27 $^5G_6$ + 0.03 $^5F_2$
	109	Γ_1		21490	82.04 $^5F_2$+14.10 $^3K_8$ + 3.02 $^5F_3$
	110	Γ_1		21510	99.76 $^3K_8$ + 0.12 $^5G_6$ + 0.09 $^5F_2$
	111	Γ_2		21519	99.77 $^3K_8$ + 0.19 $^5G_6$ + 0.01 $^3G_5$
	112	Γ_1		21530	98.57 $^3K_8$ + 1.03 $^5F_2$ + 0.33 $^5G_6$
	113	Γ_1		21547	99.79 $^3K_8$ + 0.11 $^5G_6$ + 0.07 $^5F_2$
	114	Γ_2		21577	99.40 $^3K_8$ + 0.54 $^5G_6$ + 0.04 $^5F_3$
	115	Γ_1		21583	99.56 $^3K_8$ + 0.39 $^5G_6$ + 0.03 $^5F_3$

Table 33 (cont'd). Predicted energy levels for Ho^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
116	Γ_2		21602	$99.77\,^3K_8 + 0.19\,^5G_6 + 0.01\,^5F_3$
117	Γ_2		21606	$99.76\,^3K_8 + 0.20\,^5G_6 + 0.01\,^3G_5$
118	Γ_1		21640	$99.36\,^3K_8 + 0.56\,^5G_6 + 0.04\,^5F_2$
119	Γ_1		21641	$99.48\,^3K_8 + 0.43\,^5G_6 + 0.08\,^5F_2$
120	Γ_1	$^5G_6$	22141	$97.52\,^5G_6 + 0.59\,^3K_8 + 0.52\,^5F_4$
121	Γ_2	22094	22154	$97.99\,^5G_6 + 0.50\,^5F_4 + 0.40\,^3G_5$
122	Γ_1	$^5F_1$	22160	$97.76\,^5G_6 + 0.57\,^3K_8 + 0.37\,^5F_2$
123	Γ_2	22375	22170	$97.53\,^5G_6 + 0.64\,^3G_5 + 0.61\,^5F_1$
124	Γ_2		22264	$97.21\,^5G_6 + 0.81\,^5F_3 + 0.59\,^3G_5$
125	Γ_1		22279	$97.05\,^5G_6 + 0.88\,^3G_5 + 0.70\,^5F_3$
126	Γ_1		22330	$97.02\,^5G_6 + 0.86\,^3G_5 + 0.62\,^5F_3$
127	Γ_2		22426	$98.03\,^5G_6 + 0.42\,^3G_5 + 0.39\,^5F_5$
128	Γ_2		22478	$97.65\,^5G_6 + 0.41\,^5F_5 + 0.40\,^5F_1$
129	Γ_1		22480	$57.93\,^5F_1 + 39.88\,^5G_6 + 1.09\,^3G_5$
130	Γ_1		22512	$90.39\,^5G_6 + 7.94\,^5F_1 + 0.77\,^3G_5$
131	Γ_1		22545	$71.57\,^5G_6 + 27.04\,^5F_1 + 0.68\,^3G_5$
132	Γ_2		22554	$96.83\,^5G_6 + 1.72\,^5F_1 + 0.71\,^3G_5$
133	Γ_1		22557	$94.25\,^5G_6 + 4.49\,^5F_1 + 0.27\,^5F_2$
134	Γ_2		22673	$95.73\,^5F_1 + 1.67\,^5G_6 + 1.59\,^5F_2$
135	Γ_2		22723	$97.27\,^5F_1 + 1.19\,^5G_6 + 0.71\,^5F_2$
136	Γ_1	$^3G_5$	24018	$98.73\,^3G_5 + 0.45\,^5F_3 + 0.29\,^5G_6$
137	Γ_2	23887	24023	$98.99\,^3G_5 + 0.34\,^5F_3 + 0.34\,^5F_2$
138	Γ_1		24079	$98.83\,^3G_5 + 0.55\,^5G_6 + 0.30\,^5F_3$
139	Γ_2		24088	$99.19\,^3G_5 + 0.30\,^5G_6 + 0.26\,^5F_3$
140	Γ_2		24103	$98.31\,^3G_5 + 0.99\,^5G_6 + 0.21\,^5F_3$
141	Γ_1		24163	$99.00\,^3G_5 + 0.69\,^5G_6 + 0.11\,^5F_4$
142	Γ_2		24177	$98.31\,^3G_5 + 1.32\,^5G_6 + 0.23\,^5F_3$
143	Γ_1		24204	$97.87\,^3G_5 + 1.42\,^5G_6 + 0.34\,^5F_2$
144	Γ_1		24212	$97.50\,^3G_5 + 1.83\,^5G_6 + 0.26\,^5F_2$
145	Γ_2		24293	$99.42\,^3G_5 + 0.26\,^5G_6 + 0.11\,^5F_5$
146	Γ_2		24296	$99.27\,^3G_5 + 0.39\,^5G_6 + 0.11\,^5F_5$

^{a}Aqueous centroids (cm^{-1}).

Table 34. Predicted energy levels for Tm^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	Γ_1	$^3H_6$	0	$99.61\,^3H_6 + 0.33\,^3F_4 + 0.02\,^3H_4$
2	Γ_2	202	9	$99.65\,^3H_6 + 0.29\,^3F_4 + 0.02\,^3F_3$
3	Γ_2		143	$99.49\,^3H_6 + 0.45\,^3F_4 + 0.02\,^3H_4$
4	Γ_1		145	$99.63\,^3H_6 + 0.29\,^3F_4 + 0.03\,^3H_5$
5	Γ_2		292	$99.89\,^3H_6 + 0.06\,^3H_5 + 0.04\,^3F_4$
6	Γ_1		373	$99.77\,^3H_6 + 0.16\,^3F_4 + 0.05\,^3H_5$
7	Γ_1		406	$99.83\,^3H_6 + 0.09\,^3F_4 + 0.06\,^3H_5$
8	Γ_2		513	$99.72\,^3H_6 + 0.25\,^3F_4 + 0.02\,^3H_4$
9	Γ_1		534	$99.51\,^3H_6 + 0.43\,^3F_4 + 0.03\,^3H_4$
10	Γ_2		691	$99.86\,^3H_6 + 0.07\,^3H_5 + 0.05\,^3F_4$
11	Γ_2		726	$99.80\,^3H_6 + 0.11\,^3F_4 + 0.06\,^3H_5$
12	Γ_1		1090	$99.71\,^3H_6 + 0.24\,^3F_4 + 0.03\,^3H_5$
13	Γ_1		1092	$99.72\,^3H_6 + 0.23\,^3F_4 + 0.03\,^3H_5$

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
14	Γ_1	$^3F_4$	5805	$99.45\,^3F_4 + 0.28\,^3H_6 + 0.12\,^3H_5$
15	Γ_2	5812	5867	$99.23\,^3F_4 + 0.34\,^3H_6 + 0.32\,^3H_5$
16	Γ_1		5892	$99.18\,^3F_4 + 0.44\,^3H_5 + 0.28\,^3H_6$
17	Γ_2		5994	$98.97\,^3F_4 + 0.85\,^3H_5 + 0.16\,^3H_6$
18	Γ_2		6096	$99.59\,^3F_4 + 0.23\,^3H_5 + 0.10\,^3H_6$
19	Γ_1		6244	$98.83\,^3F_4 + 0.69\,^3H_5 + 0.34\,^3H_6$
20	Γ_1		6263	$99.42\,^3F_4 + 0.28\,^3H_6 + 0.16\,^3H_5$
21	Γ_1		6298	$98.75\,^3F_4 + 0.63\,^3H_6 + 0.51\,^3H_5$
22	Γ_2		6338	$98.84\,^3F_4 + 0.59\,^3H_6 + 0.43\,^3H_5$
23	Γ_2	$^3H_5$	8258	$98.76\,^3H_5 + 0.77\,^3F_4 + 0.18\,^3H_4$
24	Γ_1	8390	8264	$99.09\,^3H_5 + 0.50\,^3F_4 + 0.25\,^3F_3$
25	Γ_1		8404	$98.68\,^3H_5 + 0.74\,^3F_4 + 0.34\,^3H_4$
26	Γ_2		8458	$99.33\,^3H_5 + 0.42\,^3F_3 + 0.13\,^3H_4$
27	Γ_2		8547	$99.38\,^3H_5 + 0.28\,^3H_4 + 0.24\,^3F_4$
28	Γ_2		8682	$99.42\,^3H_5 + 0.26\,^3F_4 + 0.25\,^3F_3$
29	Γ_1		8685	$99.14\,^3H_5 + 0.42\,^3F_4 + 0.32\,^3F_3$
30	Γ_1		8781	$99.40\,^3H_5 + 0.19\,^3H_4 + 0.15\,^3F_4$
31	Γ_1		8796	$99.52\,^3H_5 + 0.16\,^3H_4 + 0.13\,^3F_4$
32	Γ_2		9186	$99.34\,^3H_5 + 0.24\,^3F_4 + 0.24\,^3H_4$
33	Γ_2		9189	$99.30\,^3H_5 + 0.26\,^3F_4 + 0.22\,^3H_4$
34	Γ_2	$^3H_4$	12685	$97.03\,^3H_4 + 2.49\,^3F_3 + 0.24\,^3F_2$
35	Γ_1	12720	12751	$97.81\,^3H_4 + 1.65\,^3F_3 + 0.43\,^3F_2$
36	Γ_1		12758	$98.02\,^3H_4 + 1.42\,^3F_2 + 0.20\,^3F_3$
37	Γ_2		12911	$97.31\,^3H_4 + 1.94\,^3F_2 + 0.36\,^3F_3$
38	Γ_1		12990	$98.73\,^3H_4 + 0.57\,^3F_2 + 0.39\,^3F_3$
39	Γ_2		12993	$99.39\,^3H_4 + 0.38\,^3H_5 + 0.12\,^3F_3$
40	Γ_1		13081	$98.88\,^3H_4 + 0.51\,^3F_3 + 0.32\,^3H_5$
41	Γ_1		13283	$97.43\,^3H_4 + 1.91\,^3F_3 + 0.27\,^3F_2$
42	Γ_2		13309	$96.97\,^3H_4 + 2.38\,^3F_3 + 0.31\,^3F_2$
43	Γ_2	$^3F_3$	14677	$99.03\,^3F_3 + 0.66\,^3H_4 + 0.22\,^3H_5$
44	Γ_2	14510	14719	$97.09\,^3F_3 + 1.54\,^3H_4 + 1.15\,^3F_2$
45	Γ_1		14794	$95.52\,^3F_3 + 2.13\,^3H_4 + 2.01\,^3F_2$
46	Γ_1		14818	$91.94\,^3F_3 + 5.64\,^3F_2 + 2.19\,^3H_4$
47	Γ_2		14860	$96.63\,^3F_3 + 3.17\,^3F_2 + 0.09\,^3H_4$
48	Γ_1		14897	$88.59\,^3F_3 + 9.72\,^3F_2 + 1.13\,^3H_4$
49	Γ_2		14914	$97.80\,^3F_3 + 1.21\,^3H_4 + 0.59\,^3H_5$
50	Γ_1	$^3F_2$	15196	$97.65\,^3F_2 + 1.29\,^3F_3 + 0.81\,^3H_4$
51	Γ_1	15116	15342	$87.25\,^3F_2 + 11.27\,^3F_3 + 1.28\,^3H_4$
52	Γ_2		15488	$94.12\,^3F_2 + 3.30\,^3F_3 + 2.21\,^3H_4$
53	Γ_1		15608	$93.97\,^3F_2 + 3.65\,^3F_3 + 2.03\,^3H_4$
54	Γ_2		15638	$98.19\,^3F_2 + 1.32\,^3F_3 + 0.29\,^3H_4$
55	Γ_1	$^1G_4$	21212	$99.78\,^1G_4 + 0.05\,^1I_6 + 0.05\,^1D_2$
56	Γ_2	21374	21263	$99.83\,^1G_4 + 0.05\,^3F_3 + 0.04\,^1I_6$
57	Γ_1		21391	$99.75\,^1G_4 + 0.08\,^1D_2 + 0.06\,^1I_6$
58	Γ_2		21577	$99.87\,^1G_4 + 0.09\,^1I_6 + 0.01\,^3H_4$
59	Γ_2		21614	$99.81\,^1G_4 + 0.11\,^1D_2 + 0.03\,^3F_2$
60	Γ_1		21781	$99.58\,^1G_4 + 0.17\,^1I_6 + 0.15\,^1D_2$
61	Γ_2		21869	$99.64\,^1G_4 + 0.16\,^1D_2 + 0.11\,^1I_6$
62	Γ_1		22041	$99.81\,^1G_4 + 0.05\,^1I_6 + 0.04\,^3H_4$
63	Γ_1		22045	$99.85\,^1G_4 + 0.05\,^1I_6 + 0.03\,^3H_4$

Table 34 (cont'd). Predicted energy levels for Tm^{3+} in $Ca_5(PO_4)_3F$, C_s site. B_{nm} from table 9.

Table 34 (cont'd). Predicted energy levels for Tm^{3+} in Ca$_5$(PO$_4$)$_3$F, C_s site. B_{nm} from table 9.

Level	I. R.	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
64	Γ_1	$^1D_2$	28104	99.78 $^1D_2$ + 0.07 $^1G_4$ + 0.05 $^1I_6$
65	Γ_1	28032	28135	99.70 $^1D_2$ + 0.13 $^1G_4$ + 0.05 $^3F_2$
66	Γ_2		28379	99.33 $^1D_2$ + 0.31 $^3P_1$ + 0.21 $^1G_4$
67	Γ_2		28433	99.54 $^1D_2$ + 0.19 $^3P_1$ + 0.08 $^1G_4$
68	Γ_1		28557	99.69 $^1D_2$ + 0.13 $^1G_4$ + 0.03 $^3P_0$
69	Γ_1	$^1I_6$	34407	99.75 $^1I_6$ + 0.12 $^1G_4$ + 0.08 $^3P_2$
70	Γ_2	34886	34408	99.82 $^1I_6$ + 0.12 $^1G_4$ + 0.03 $^3P_2$
71	Γ_2	$^3P_0$	34574	99.87 $^1I_6$ + 0.08 $^3P_2$ + 0.03 $^1G_4$
72	Γ_1	35637	34587	99.84 $^1I_6$ + 0.10 $^3P_2$ + 0.02 $^1G_4$
73	Γ_1		34799	99.79 $^1I_6$ + 0.09 $^3P_2$ + 0.07 $^1G_4$
74	Γ_2		34917	99.66 $^1I_6$ + 0.23 $^3P_2$ + 0.05 $^1D_2$
75	Γ_2		34981	99.96 $^1I_6$ + 0.02 $^1G_4$ + 0.01 $^3P_2$
76	Γ_1		35277	99.51 $^1I_6$ + 0.33 $^3P_0$ + 0.11 $^3P_2$
77	Γ_1		35312	99.85 $^1I_6$ + 0.07 $^3P_2$ + 0.05 $^1G_4$
78	Γ_2		35852	99.84 $^1I_6$ + 0.10 $^3P_2$ + 0.03 $^3P_1$
79	Γ_2		35864	99.90 $^1I_6$ + 0.04 $^3P_2$ + 0.03 $^1G_4$
80	Γ_1		35911	97.65 $^3P_0$ + 1.21 $^3P_2$ + 0.99 $^1I_6$
81	Γ_1		36146	99.73 $^1I_6$ + 0.14 $^3P_2$ + 0.06 $^3P_1$
82	Γ_1		36151	99.14 $^1I_6$ + 0.62 $^3P_0$ + 0.13 $^3P_2$
83	Γ_1	$^3P_1$	36315	99.59 $^3P_1$ + 0.18 $^3P_2$ + 0.12 $^1I_6$
84	Γ_2	36298	36652	96.99 $^3P_1$ + 2.60 $^3P_2$ + 0.30 $^1D_2$
85	Γ_2		36798	98.72 $^3P_1$ + 0.95 $^3P_2$ + 0.20 $^1D_2$
86	Γ_1	$^3P_2$	38066	99.51 $^3P_2$ + 0.32 $^1I_6$ + 0.08 $^3P_1$
87	Γ_1	38193	38269	99.51 $^3P_2$ + 0.29 $^1I_6$ + 0.10 $^3P_1$
88	Γ_2		38520	97.06 $^3P_2$ + 2.61 $^3P_1$ + 0.24 $^1I_6$
89	Γ_1		38759	98.60 $^3P_2$ + 1.19 $^3P_0$ + 0.10 $^1I_6$
90	Γ_2		38976	98.74 $^3P_2$ + 0.98 $^3P_1$ + 0.19 $^1I_6$
91	Γ_1	$^1S_0$ 79592	79891	99.97 $^1S_0$ + 0.01 $^3P_2$ + 0.01 $^1G_4$

^{a}Aqueous centroids (cm^{-1}).

Table 35. Predicted energy levels for Yb^{3+} in Ca$_5$(PO$_4$)$_3$F C_s site. B_{nm} from table 9.

Level	$[(S,L)J]^a$	Energy (cm^{-1})	Free ion mixture (%)
1	$^2F_{7/2}$	0	99.94 $^2F_{7/2}$ + 0.06 $^2F_{5/2}$
2	250	186	99.96 $^2F_{7/2}$ + 0.04 $^2F_{5/2}$
3		702	99.92 $^2F_{7/2}$ + 0.08 $^2F_{5/2}$
4		1036	99.98 $^2F_{7/2}$ + 0.02 $^2F_{5/2}$
5	$^2F_{5/2}$	10217	99.96 $^2F_{5/2}$ + 0.04 $^2F_{7/2}$
6	10450	10694	99.90 $^2F_{5/2}$ + 0.10 $^2F_{7/2}$
7		11169	99.94 $^2F_{5/2}$ + 0.06 $^2F_{7/2}$

^{a}Aqueous centroids (cm^{-1}).

5. Conclusion

The results of analyzing the optical spectra of Er^{3+} in the two Ca^{2+} sites in $Ca_5(PO_4)_3F$ have been used in the derivation of two sets of crystal-field parameters for the entire series of rare-earth ions, Ln^{3+}. These crystal-field parameters were then used to predict the energy levels of these ions in each of the two different sites: Ca1 (C_3 symmetry) and Ca2 (C_s symmetry). The very large values of the crystal fields (especially the B_{2m} components) cause a very severe mixing of the higher crystal-field energy levels. The mixing is so severe in many of the ions that it precludes completely any purely experimental attempts to analyze the data by analogy to known spectra taken in host materials where the crystal field is much weaker. I hope that the results presented here will serve as a rough guide to experimenters in attempts to unravel their experimental data. In addition to the energy levels, I have used the point-charge model to evaluate the crystal-field components, A_{nm}, and thereby obtained estimates of the Judd-Ofelt intensity parameters, Ω_k. The energy-level eigenfunctions have been used to predict the Zeeman g factors for both sites. These latter quantities may also serve as aids in the interpretation of the experimental data.

References

1. R.W.G. Wyckoff, *Crystal Structures*, **3**, Interscience (1965), 228.

2. J. M. Hughes, M. Cameron, and K. D. Crowley, *Structural Variations in Natural F, OH, and Cl Apatites*, Am. Mineral. **74** (1989), 870.

3. D. L. Dexter, *A Theory of Sensitized Luminescence in Solids*, J. Chem. Phys. **21** (1953), 836.

4. C. A. Morrison, *Angular Momentum Theory Applied to Interactions in Solids*, Lecture Notes in Chemistry **47**, Springer-Verlag (1988).

5. C. A. Morrison and R. P. Leavitt, *Crystal-Field Analysis of Triply Ionized Rare-Earth Ions in Lanthanum Trifluoride*, J. Chem. Phys. **71** (1979), 2366. (The $\rho_4(Gd) = 0.4490$ Å^4, not 0.4990 Å^4, as given in table II.)

6. C. A. Morrison and R. P. Leavitt, "Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Materials," in Volume 5, *Handbook of the Physics and Chemistry of Rare Earths*, ed. by K. A. Gschneidner, Jr., and L. Eyring, North-Holland Publishers, New York, NY (1982).

7. T. H. Allik, C. A. Morrison, J. B. Gruber, and M. R. Kokta, *Crystallography, Spectroscopic Analysis, and Lasing Properties of Nd^{3+}:$Y_3Sc_2Al_3O_{12}$*, Phys. Rev. **B41** (1990), 21.

8. N. C. Chang, J. B. Gruber, R. P. Leavitt, and C. A. Morrison, *Optical Spectra, Energy Levels, and Crystal-Field Analysis of Tripositive Rare-Earth Ions in Y_2O_3. I. Kramers Ions in C_2 Sites*, J. Chem. Phys. **76** (1982), 3877. See also C. A. Morrison, R. P. Leavitt, and D. E. Wortman, *Crystal-Field Analysis of Triply Ionized Lanthanides in $CS_2NaLnCl_6$*, J. Chem. Phys. **73** (1980), 2580.

9. G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups*, MIT Press, Cambridge, MA (1963).

10. J. B. Gruber, M. D. Seltzer, M. E. Hills, T. H. Allik, J. A. Hutchinson, C. A. Morrison, and B.H.T. Chai, *Site-Selective Spectra and Energy Levels of Trivalent Erbium in Calcium Fluorophosphate*, Opt. Mat. **3** (1994), 99.

11. R. P. Leavitt and C. A. Morrison, *Crystal-Field Analysis of Triply Ionized Rare-Earth Ions in Lanthanum Trifluoride. II. Intensity Calculations*, J. Chem. Phys. **73** (1980), 749.

Appendix A. Selection Rules for Dipole Electronic Transitions in $Ca_5(PO_4)_3F$

Contents

Tables

The electric dipole operator, **p**, interacting with an external electric field, **E**, gives rise to the Hamiltonian

$$H^{ed} = -\mathbf{p} \cdot \mathbf{E} \quad , \tag{A-1}$$

where

$$\mathbf{p} = -e \sum_i \mathbf{r}_i \quad . \tag{A-2}$$

For the magnetic dipole, the interaction with an external magnetic field H is

$$H^{md} = e \left(\frac{\alpha_o}{2} \right) \mathbf{m} \cdot \mathbf{H} \quad , \tag{A-3}$$

where

$$\mathbf{m} = \mathbf{L} + g_e \mathbf{S} \, , \tag{A-4}$$

and **L** is the total orbital angular momentum, **S** is the total spin angular momentum, g_e is the free electron g factor, and α_o is the fine structure constant. For ions occupying either of the sites Ca1 or Ca2 in fluoroapatite, the principal axis is the c-axis of the crystal, which I take as the z-axis in the following. The two types of polarization data, $\mathbf{k} \perp z$ and $\mathbf{k} \parallel z$, with **k** the direction of propagation of the fields **E** and **H**, are referred to simply as the polarization spectra and the axial spectra. The axial spectra arise where $\mathbf{k} \parallel z$ (note that I am considering only propagation along the principal axis so that $\mathbf{k} \cdot \mathbf{E} = \mathbf{k} \cdot \mathbf{H} = 0$). The result with $\mathbf{E} \parallel z$ is referred to as π and with $\mathbf{E} \perp z$ is referred to as σ. (This labeling always refers to the E vector even for magnetic dipole transitions.)

A-1. C_3 Symmetry Site (Ca1)

A-1.1 Electric Dipole in C_3 Symmetry

The electric dipole interaction can be written

$$H^{ed} = e\left(xE_x + yE_y + zE_z\right) , \qquad (A\text{-}5)$$

where x represents the total x component of $\Sigma_i r_i$ and y and z represent similar abbreviations. From table 42, page 51 of Koster et al[1] (I refer to the tables and pages in this reference in all the following), we have the following:

$$x \rightarrow \Gamma_2 + \Gamma_3 ,$$

$$y \rightarrow \Gamma_2 + \Gamma_3 , \qquad (A\text{-}6)$$

$$z \rightarrow \Gamma_1 ,$$

and from the group multiplication (Koster et al, table 43), we have the result given in table A-1 for the four types of experimental arrangement. In C_3 symmetry, the Γ_2 and Γ_3 irreducible representations are degenerate, and we label them $\Gamma_{2,3}$. Similarly, for the Γ_4 and Γ_5, we label them $\Gamma_{4,5}$.

Table A-1. Allowed electric dipole transitions for $4f^N$ electronic configuration in C_3 symmetry.

(a) N even (J integer)
$(\mathbf{k} \perp z)$[a]

	Γ_1	$\Gamma_{2,3}$
Γ_1	π	σ
$\Gamma_{2,3}$	σ	π, σ

$(\mathbf{k} \parallel z)$[a]

	Γ_1	$\Gamma_{2,3}$
Γ_1	0	σ
$\Gamma_{2,3}$	σ	σ

(b) N odd (J half integer)
$(\mathbf{k} \perp z)$[b]

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	π, σ	σ
Γ_6	σ	π

$(\mathbf{k} \parallel z)$[b]

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	σ	σ
Γ_6	σ	0

[a]Applicable to the following tables in the main body: 14, 16, 18, 20, 22, 23.
[b]Applicable to the following tables in the main body: 5, 13, 15, 17, 19, 21, 24.

[1]G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups*, MIT Press, Cambridge, MA (1963).

A-1.2   Magnetic Dipole in C_3 Symmetry

The magnetic dipole interaction can be written

$$H^{md} = e\left(\frac{\alpha_0}{2}\right)\left(m_x H_x + m_y H_y + m_z H_z\right) , \qquad (A\text{-}7)$$

and again (table 42, page 51 of Koster et al), we have

$$m_x \rightarrow \Gamma_2 + \Gamma_3 ,$$

$$m_y \rightarrow \Gamma_2 + \Gamma_3 , \qquad (A\text{-}8)$$

$$m_z \rightarrow \Gamma_1$$

(m_i is read as S_i in table 42). Using the multiplication table given in table 43 of Koster et al, we obtain the result given in table A-2.

Table A-2. Allowed magnetic dipole transitions for $4f^N$ electronic configuration in C_3 symmetry.

(a) *N* even (*J* integer)

$(k \perp z)^a$

	Γ_1	$\Gamma_{2,3}$
Γ_1	σ	π
$\Gamma_{2,3}$	π	σ, π

$(k \parallel z)^a$

	Γ_1	$\Gamma_{2,3}$
Γ_1	0	σ
$\Gamma_{2,3}$	σ	σ

(b) *N* odd (*J* half integer)

$(k \perp z)^b$

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	π, σ	π
Γ_6	π	σ

$(k \parallel z)^b$

	$\Gamma_{4,5}$	Γ_6
$\Gamma_{4,5}$	σ	σ
Γ_6	σ	0

[a]Applicable to the following tables in the main body: 14, 16, 18, 20, 22, 23.

[b]Applicable to the following tables in the main body: 5, 13, 15, 17, 19, 21, 24.

A-2. C_s Symmetry Site (Ca2)

A-2.1 Electric Dipole in C_s Symmetry

In C_s symmetry, the components of the electric dipole interaction given in equation (A-5) transform as

$$x \rightarrow \Gamma_1 ,$$

$$y \rightarrow \Gamma_1 ,$$

$$z \rightarrow \Gamma_2 ,$$

(A-9)

given in table 9, page 33, of Koster et al. Using equation (A-9) and the multiplication table given in table 10 of Koster et al, we obtain the results given in table A-3.

Table A-3. Allowed electric dipole transitions for $4f^N$ electronic configuration in C_s symmetry.

(a) N even (J integer)

$(k \perp z)^a$

	Γ_1	Γ_2
Γ_1	σ	π
Γ_2	π	σ

$(k \parallel z)^a$

	Γ_1	Γ_2
Γ_1	σ	0
Γ_2	0	σ

(b) N odd (J half integer) [b]

$(k \perp z)^c$

	Γ_3	Γ_4
Γ_3	σ	π
Γ_4	π	σ

$(k \parallel z)^c$

	Γ_3	Γ_4
Γ_3	σ	0
Γ_4	0	σ

[a]Applicable to the following tables in the main body: 26, 28, 30, 32, 34, 35.

[b]In the double C_s group, the energy levels are all in the degenerate Kramer's doublet $\Gamma_3 + \Gamma_4$, but the tables are useful in the study of the Zeeman effect.

[c]Applicable to the following tables in the main body: 6, 25, 27, 29, 31, 33, 36.

A-2.2 Magnetic Dipole in C_s Symmetry

The magnetic dipole interaction given in equation (A-3) has components that transform in C_s symmetry as

$$m_x \rightarrow \Gamma_2 \, ,$$

$$m_y \rightarrow \Gamma_2 \, , \qquad\qquad (A\text{-}10)$$

$$m_z \rightarrow \Gamma_1 \, ,$$

from table 9, page 33, of Koster et al. Using the multiplication table (again the π and σ refer to the *electric vector* being parallel or perpendicular to the z-axis, respectively), we obtain the result given in table A-4.

Table A-4. Allowed magnetic dipole transitions for $4f^N$ electronic configuration in C_s symmetry.

(a) *N* even (*J* integer)

$(k \perp z)$[a]

	Γ_1	Γ_2
Γ_1	σ	π
Γ_2	π	σ

$(k \parallel z)$[a]

	Γ_1	Γ_2
Γ_1	0	σ
Γ_2	σ	0

(b) *N* odd (*J* half integer)[b]

$(k \perp z)$[c]

	Γ_3	Γ_4
Γ_3	σ	π
Γ_4	π	σ

$(k \parallel z)$[c]

	Γ_3	Γ_4
Γ_3	0	σ
Γ_4	σ	0

[a]Applicable to the following tables in the main body: 26, 28, 30, 32, 34, 35.

[b]In the double C_s group, the energy levels are all in the degenerate doublet $\Gamma_3 + \Gamma_4$, but the tables are useful in the study of the Zeeman effect.

[c]Applicable to the following tables in the main body: 6, 25, 27, 29, 31, 33, 36.

Appendix B. Bibliography of Articles on Fluoroapatites

$Ca_5(PO_4)_5F$, investigated in the main body of this report, is one of the fluoroapatites, a subgroup of the apatites. The fluoroapatites are the most stable and practical apatites for use in lasers and fluorescent light sources. The following bibliography provides a range of references on this useful group.

Abdulsabirov, R. Yu., and I. N. Kurkin, Parameters of a Crystalline Field at Ca II Positions in Single Crystals of Fluoroapatite, Opt. Spectrosc. **32** (1971), 324.

Aleksandrov, V. I., A. A. Kaminskii, G. V. Maksimova, A. M. Prokhorov, S. E. Sarkisov, A. A. Sobol´, and V. M. Tatarintsev, *Stimulated Radiation of Nd^{3+} Ions in Crystals for the $^4F_{3/2} \rightarrow {}^4I_{13/2}$ Transition*, Sov. Phys. Dokl. **18** (1974), 495.

Altchuler, Z. S., S. Berman, and F. Cuttitta, *Rare Earths in Phosphorites—Geochemistry and Potential Recovery*, US Geol. Surv., Prof. Paper 575-b (1967).

Anderson, J. B., and E. Kostiner, *The Crystal Structure of Cobalt-Substituted Calcium Chlorapatite*, J. Solid State Chem. **66** (1987), 343.

Avanesov, A. G., T. T. Basiev, Yu. K. Voron´ko, B. I. Denker, G. C. Maksimova, V. A. Myzina, V. V. Osiko, and V. S. Fedorov, *Investigation of Spatial Distribution of Impurities in Solids by the Method of Kinetic Luminescent Spectroscopy*, Sov. Phys. JETP **57** (1983), 596.

Bhatnagar, V. M., *The Cell Parameters of Synthetic Calcium Apatites*, Rev. Roumaine Chim. **15** (1970), 1735.

Bhatnager, V. M., *Preparation and X-Ray Powder Diffraction Patterns of Lead Apatites*, Chem. Ind. (London) **48** (1970), 1538.

Bhatnager, V. M., *The Cell Parameters of Synthetic Fluorapatite, Ca$_{10}$(PO$_4$)$_6$F$_2$*, Rev. Roumaine Chim. **15** (1970), 87.

Bhatnager, V. M., *The Melting Points of Synthetic Apatites*, Mineral. Mag. **37** (1968), 527.

Daraseliya, D. M., G. V. Maksimov, and A. A. Manenkov, *Relaxation Processes and Discrete Saturation Effects in the EPR Spectrum of Nd^{3+} in Ca$_5$(PO$_4$)$_3$F*, JETP Lett. **10** (1969), 229.

DeLoach, L. D., S. A. Payne, L. K. Smith, W. L. Kway, and W. F. Krupke, *Laser and Spectroscopic Properties of Sr$_5$(PO$_4$)$_3$F:Yb*, J. Opt. Soc. Am. **B11** (1994), 269.

Elliott, J. C., *Recent Progress in the Chemistry, Crystal Chemistry and Structure of the Apatites*, Calc. Tissue Res. **3** (1969), 293.

Engel, G., *Einige Cadmiumapatite Sowie die Verbindungen Cd$_2$XO$_4$F mit X = P, As und V*, Zeits. Anorg. Allg. Chem. **378** (1970), 49.

Engel, G., *Hydrothermalsynthese von Bleihydroxylapatiten Pb$_5$(XO$_4$)OH mit X = P, As, V*, Naturwiss. **57** (1970), 355.

Federov, N. F., I. F. Andreev, A. M. Shevjokov, and T. A. Tunik, *Silicoapatites of Sr and Nb*, Izvest. Akad. Nauk SSSR, Neorg. Mater. **6** (1970), 2018.

Felsche, J., *A New Cerium (III) Orthosilicate with the Apatite Structure*, Naturwiss. **56** (1969), 325.

Fleet, M.E., and Y. Pan, *Site Preference of Nd in Fluorapatite [Ca$_{10}$(PO$_4$)$_6$F$_2$]*, J. Solid State Chem. **112** (1994), 78.

Foreman, D. W., Jr., *Neutron and X-Ray Diffraction Study of $Ca_3Al_2(O_4D_4)_3$, a Garnetoid,* Chem. Phys. **48** (1968), 3037.

Grisafe, D. A., and F. A. Hummel, *Pentavalent Ion Substitutions in the Apatite Structure. Part A. Crystal Chemistry,* J. Solid State Chem. **2** (1970), 160.

Johnson, P. D., J. S. Prener, and J. D. Kingsley, *Apatite: Origin of Blue Color,* Science **141** (1963), 1179.

Johnson, W., *Two Synthetic Compounds Containing Chromium in Different Valency States,* Mineral. Mag. **32** (1960), 408.

Kaplyanskii, A. A., and E. G. Kuzminov, *Piezospectroscopic Effect and Local-Field Symmetry in Neodymium-Doped Fluorapatite Crystals,* Opt. Spektrosk. **29** (1970), 706 [trans. Opt. Spectrosc. **29** (1970), 376].

Kaplyanskii, A. A., V. N. Medvedev, and A. P. Skvortsov, *Linear Stark Effect in the Spectra of Fluorapatite Crystals Activated by Rare-Earth Ions,* Opt. Spektrosk. **36** (1974), 368 [trans. Opt. Spectrosc. **36** (1974), 213].

Klee, W. E., *The Vibrational Spectra of the Phosphate Ions in Fluorapatite,* Zeits. Kristallogr. **131** (1970), 95.

Klee, W. E., and G. Engel, *I. R. Spectra of the Phosphate Ions in Various Apatites,* J. Inorg. Nucl. Chem. **32** (1970), 1837.

Klement, R., *Natrium-Calcium-Sulfapatite $Na_6Ca_4(SO_4)_6F_2$,* Naturwiss. **27** (1939), 568.

Larsen, E. S., Jr., M. H. Fletcher, and E. A. Cisney, *Strontian Apatite,* Am. Mineral. **37** (1952), 656.

Lavat, A. E., S. B. Etcheverry, and E. J. Baran, *Crystallographic and Spectroscopic Behavior of Some Mixed Phosphate Vanadate Fluoroapatite,* Z. Naturforsch. **41b** (1986), 987 [in German].

Levitt, S. R., and R. A. Condrate, Sr., *The Vibrational Spectra of Lead Apatites,* Am. Mineral. **55** (1970), 1562.

Maksimova, G. V., and A. A. Sobol', *Local Charge Compensation of the Nd^{3+} Ion in Fluorapatite Crystals,* Akad. Nauk SSSR Neorg. Mat. **8** (1972), 1077.

Maksimova, G. V., and A. A. Sobol', *Nd^{3+} Optical Centers in Crystals of Calcium and Strontium Fluorophosphates,* (1972) Proceedings (Trudy) of the P. N. Lebedev Physics Institute, **60**, pp 59–73.

Mayer, I., and V. Makogon-Loewy, *Eu(II)-Hydroxyapatite. Preparation and Crystal Data,* Israel J. Chem. **7** (1969), 717.

Mazelsky, R., R. H. Hopkins, and W. E. Kramer, *Czochralski-Growth of Fluorophosphate,* J. Cryst. Growth **3, 4** (1968), 360.

McConnell, D., *Infrared Absorption of Carbonate Apatite,* Science **155** (1967), 607.

McConnell, D., *Crystal Chemical Calculations,* Geochim. Cosmochim. Acta **31** (1967), 1479.

McConnell, D., *Calculation of the Unit-Cell Volume of a Complex Mineral Structure,* Zeits. Kristallogr. **123** (1966), 58.

McConnell, D., *Crystal Chemistry of Hydroxyapatite: Its Relation to Bone Mineral,* Arch. Oral. Biol. **10** (1965), 421.

McConnell, D., *Deficiency of Phosphate Ions in Apatite,* Naturwiss. **52** (1965), 183.

McConnell, D., and D. W. Foreman, Jr., *The Properties and Structure of $Ca_{10}(PO_4)_6 (OH)_2$; Its Relation to Tin (II) Apatite,* Can. Mineral. **8** (1966), 431.

Moreno, E. C., T. M. Gregory, and W. E. Brown, *Preparation and Solubility of Hydroxyapatite,* Nat. Bur. Stand. J. Res. **72A** (1968), 773.

Morozov, A. M., L. G. Morozova, A. K. Trefimov, and P. P. Feofilov, *Spectral and Luminescent Characteristics of Fluoroapatite Single Crystals Activated by Rare Earth Ions,* Opt. Spektrosk. **29** (1970), 1106 [trans. Opt. Spectrosc. **29** (1970), 590].

Ohlmann, R. C., N. T. Melamed, R. Mazelsky, and W. E. Kramer, *Sensitized Fluorescence of Rare-Earth Ions in Crystals,* Air Force Materials Laboratory, AFML-TR-67-283 (July 1967).

Prener, J. S., *The Growth and Crystallographic Properties of Calcium Fluor- and Chlor-Apatite Crystals,* J. Electrochem. Soc. **114** (1967), 77.

Proceedings of the Advanced Solid-State Laser Conference, 7–10 February 1994, Salt Lake City Utah, Opt. Soc. Am., 2010 Mass. Avenue, NW, Washington, DC 20036.

Shcherbokova, M. Y., L. G. Gilinskaya, and A. A. Godovikov, *Paramagnetic Centers in Apatite,* Kristallografiya **13** (1968), 353 [transl. **13**, 289].

Simpson, D. R., *Partitioning of Fluoride Between Solution and Apatite,* Am. Mineral. **54** (1969), 1711.

Simpson, D. R., *Substitutions in Apatite: I. Potassium-Bearing Apatite,* Am. Mineral. **53** (1968), 432.

Simpson, D. R., *Substitutions in Apatite: II. Low Temperature Fluoride-Hydroxyl Apatite,* Am. Mineral. **53** (1968), 1953.

St. Náray-Szabo, *The Structure of Apatite $(CaF)Ca_4(PO_4)_3$,* Zeits. Kristallogr. **75** (1930), 387.

Steinbruegge, K. B., T. Henningsen, R. H. Hopkins, R. Mazelsky, N. T. Melamed, E. P. Riedel, and R. C. Ohlmann, *Laser Properties of Nd^{3+} and Ho^{3+} Doped Crystals with the Apatite Structure,* Appl. Opt. **7** (1968), 905.

Trotter, J., and W. H. Barnes, *The Structure of Vanadinite,* Can. Mineral. **6** (1958), 161.

Voronko, Yu. K., G. V. Maksimova, and A. A. Sobol´, *Anisotropic Luminescence Centers of TR^{3+} Ions in Fluoroapatite Crystals,* Opt. Spectrosc. **70** (1991), 203.

Wanmaker, W. L., J. W. Ter Brugt, and J. G. Verlijskdonk, *Synthesis of New Compounds with Apatite Structure,* Phillips Res. Repts. **26** (1971), 373.

Wollentin, R. W., *Lead and Manganese-Activated Cadmium Fluorophosphate Phosphors*, J. Electrochem. Soc. **103** (1956), 17.

Yefimov, A. F., S. M. Kravchenko, and Z. V. Vasil′eva, *Strontiapatite — a New Mineral*, Dokl. Akad. Nauk **142** (1962), 439 [transl. **142**, 113].

Yoon, H. S., and R. E. Newnham, *Elastic Properties of Fluorapatite*, Am. Mineral. **54** (1969), 1193.

Zounami, A., D. Zambon, and J. C. Cousseins, *Optical Properties of Eu^{3+} Activated $Sr_{10}F_2(PO_4)_6$ Elaborated by Coprecipitation*, J. Alloys Comp. **188** (1992), 82.

Distribution

Admnstr
Defns Techl Info Ctr
Attn DTIC-DDA (2 copies)
Cameron Sta Bldg 5
Alexandria VA 22304-6145

Defns Advncd Rsrch Proj Agcy
Attn A Yang
1400 Wilson Blvd
Arlington VA 22290

Director
Defns Nuc Agcy
Attn TITL Tech Lib
6801 Telegraph Rd
Alexandria VA 22310-3398

Ofc of the Dpty Chief of Staf for Rsrch
 Dev & Acqstn
Attn DAMA-ARZ-B I R Hershner
Dept of the Army
Washington DC 20310

Under Secy of Defns Rsrch & Engrg
Attn Techl Lib 3C128
Washington DC 20301

Commander
Atmospheric Sci Lab
Attn Techl Lib
White Sands Missile Range NM 88002-5030

Night Vsn & Electro-Optics Lab LABCOM
Attn A Pinto (2 copies)
Attn B Zandi
Attn J Daunt
Attn L Merkel
Attn R Buser
Attn Techl Lib
Attn W Tressel
FT Belvoir VA 22060

Commander
US Army Mis & Munitions Ctr & Schl
Attn AMSMI-TB Redstone Sci Info Ctr
Attn ATSK-CTD-F
Redstone Arsenal AL 35809

US Army Mtrl & Mech Rsrch Ctr
Attn SLCMT-TL Techl Lib
Watertown MA 02172

US Army Rsrch Ofc
Attn G Iafrate
Attn M Strosio
Attn M Ciftan
Attn R Guenther
PO Box 12211
Research Triangle Park NJ 07709-2211

US Army Test & Eval Cmnd
Attn D H Sliney
Attn Techl Lib
Aberdeen Proving Ground MD 21005

US Army Troop Spprt Cmnd
Attn STRNC-RTL Techl Lib
Natick MA 01762

US Frgn Sci & Techlgy Ctr
Attn AIAST-BS Basic Sci Div
Federal Office Building
Charlottesville VA 22901

Nav Rsrch Lab
Attn A Rosenbaum
Attn Code 2620 Tech Lib Br
Attn Code 5554 F Bartoli
Attn Code 5554 L Esterowitz
Attn Code 5554 R E Allen
Attn G Quarles
Attn G Risenblatt
Washington DC 20375

Nav Weapons Ctr
Attn A Wright
Attn Code 3854 M Nader
Attn Code 3854 R L Atkins
Attn DOCE343 Techl Info Dept
China Lake CA 93555

Ames Lab Dow Iowa State Univ
Attn K A Gschneidner Jr (2 copies)
Ames IA 50011

Distribution

Argonne Natl Lab
Attn W T Carnall
9700 South Cass Ave
Argonne IL 60439

Lawrence Radiation Lab
Attn M J Weber
Attn W Krupke
Attn L D DeLoach
Livermore CA 94550

Los Alamos Natl Lab
Attn E T Salesky
505 Openheimer Dr
Los Alamos NM 87544

Oak Ridge Natl Lab
Attn R G Haire
Oak Ridge TN 37839

NASA Langley Rsrch Ctr
Attn C Blair
Attn D Getteny
Attn G Armagen
Attn J Barnes
Attn M Buoncristiani
Attn N P Barnes (2 copies)
Attn P Cross
Hampton VA 23665

Natl Inst of Stand & Techlgy
Attn Lib
Gaithersburg MD 20899

Natl Oceanic & Atmospheric Adm Envir
   Rsrch Lab
Attn Lib R-51 Techl Rpt
Boulder CO 80302

Arizona State Univ Dept of Chemistry
Attn L Eyring
Tempe AZ 85281

Colorado State Univ Physics Dept
Attn S Kern
FT Collins CO 80523

Departmento de Química Fundamental &
   Departmento de Fisica
Attn A da Gama
Attn G F de Sá
Attn O L Malta
da UFPE Cidade Universitaria
50.000 Recife Pe
Brasil

Howard Univ Dept of Physics
Attn Prof V Kushamaha
25 Bryant Stret NW
Washington DC 20059

Johns Hopkins Univ Dept of Physics
Attn B R Judd
Baltimore MD 21218

Kalamazoo Colg Dept of Physics
Attn K Rajnak
Kalamazoo MI 49007

MA Inst of Techlgy Crystal Physics Lab
Attn H P Jenssen
Cambridge MA 02139

Princeton Univ Dept of Chemistry
Attn C Weaver
Attn D S McClure
Princeton NJ 08544

San Jose State Univ Dept of Physics
Attn J B Gruber
San Jose CA 95192

Seton Hall Univ Chemistry Dept
Attn H Brittain
South Orange NJ 07099

Univ of Central Florida Dept of Physics
Attn B H T Chai
Attn R E Peale
Orlando FL 32816

Univ of Connecticut Dept of Physics
Attn R H Bartram
Storrs CT 06269

Distribution

Univ of Dayton Dept of Physics
Attn S P Sinha
300 College Park
Dayton OH 45469-2350

Univ of Illinois Everitt Lab
Attn J G Eden
1406 W Green Stret
Urbana IL 61801

Univ of Michigan Dept of Physics
Attn S C Rand
Ann Arbor MI 48109

Univ of Minnesota Duluth Dept of Chemistry
Attn L C Thompson
Duluth MN 55812

Univ of South Florida Physics Dept
Attn R Chang
Attn Sengupta
Tampa FL 33620

Univ of Southern California
Attn M Birnbaum
Los Angeles CA 90089

Univ of Virginia Dept of Chemistry
Attn F S Richardson (2 copies)
Charlottesville VA 22901

Univ of Wisconsin Chemistry Dept
Attn J Wright
Madison WI 53706

Université Claude Bernard
Attn R Moncorgé
43 boulevard du 11 Novembre 1918
69622 Villeurbanne
France

UPR 210 CNRS
Attn M Faucher
Attn P Caro
Attn P Porcher
1 Place A Briand 92195 Meudon
France

Allied Signal Inc
Attn R Morris
POB 1021 R
Morristown NJ 07960

Arspc Corp
Attn N C Chang
PO Box 92957
Los Angeles CA 90009

Battelle Pac Northwest Lab Battelle Blvd
Attn N Hess
PO Box 999
Richland WA 99352

Dept of Mech Indus & Arspc Eng
Attn S Temkin
PO Box 909
Piscataway NJ 08854

Engrg Societies Lib
Attn Acqstn Dept
345 East 47th Stret
New York NY 10017

Fibertech Inc
Attn H R Verdin (3 copies)
510-A Herdon Pky
Herdon VA 22070

Hughes Aircraft Comp
Attn D Sumida
Attn MS RL65 R A McFarlane
3011 Malibu Canyon Rd
Malibu CA 90265

IBM Rsrch Div Almaden Rsrch Ctr
Attn R M Macfarlane Mail Stop K32 802(d)
650 Harry Rd
San Jose CA 95120

Inst for Low Temp & Struc Rsrch Polish
  Academy of Sci
Attn R Troc
50-950 Wroclaw PO Box 937
ul. Okolna 2
Poland

Distribution

Lawrence Berkeley Lab
Attn N Edelstein
MS 70A-1150
Berkeley CA 94720

LTV
Attn M Kock (WT-50)
PO Box 650003
Dallas GX 75265

Martin Marietta
Attn F Crowne
Attn J Little
Attn P Caldwell
Attn T Worchesky
1450 South Rolling Rd
Baltimore MD 21227

McDonnell Douglass Elect Sys Comp
Attn Dept Y440 Bldg 101 Lev 2Rm/PTB54
  D M Andrauskas MS-2066267
PO Box 516
ST Louis MO 63166

MIT Lincoln Lab
Attn B Aull
PO Box 73
Lexington MA 02173

Montana Analytic Services
Attn M Schwan
325 Icepond Rd
Bozeman MT 59715

Sci Applctn Intrntl Corp
Attn T Allik
1710 Goodridge Dr
McLean VA 22102

Southwest Rsrch Inst
Attn M J Sablik
PO Drawer 28510
San Antonio TX 78228-0510

Swartz Electro-Optic Inc
Attn G A Rines
45 Winthrop Stret
Concord MA 01742

Union Carbide Corp
Attn M R Kokta
50 South 32nd Stret
Washougal WA 98671

Univ of Toronto Dept of Physics
Attn D May
Toronto Ontario MSS1A7
Canada

W J Schafer Assoc
Attn J W Collins
321 Ballerica Rd
Chelmsford MA 01824

US Army Rsrch Lab
Attn AMSRL-PS C Thornton
Attn AMSRL-PS M Thompsett
Attn AMSRL-PS T Aucoin
FT Monmouth NJ 07703-5601

US Army Rsrch Lab
Attn AMSRL-PS-AA C Morrison
  (10 copies)
Attn AMSRL-PS-AA D Wortman
  (10 copies)
Attn AMSRL-PS-AA G Simonis
Attn AMSRL-PS-AA J Bradshaw
Attn AMSRL-PS-AA J Bruno
Attn AMSRL-PS-AA J Pham
Attn AMSRL-PS-AA M Stead
Attn AMSRL-PS-AA M Tobin
Attn AMSRL-PS-AA R Leavitt
Attn AMSRL-PS-AA R Tober
Attn AMSRL-PS-AA T Bahder
Attn AMSRL-OP-SD-TA Mail & Records
  Mgmt

Distribution

US Army Rsrch Lab (cont'd)
Attn AMSRL-OP-SD-TL Tech Library
  (3 copies)
Attn AMSRL-OP-SD-TP Tech Pub
Attn AMSRL-SS-FA G Turner
Attn AMSRL-SE-RU B Zabludowski
Attn AMSRL-SE-EO C Garvin
Attn AMSRL-SEE-EO J Goff

US Army Rsrch Lab (cont'd)
Attn AMSRL-SSE-RM (A) Chf
Attn AMSRL-SE-RU A A Bencivenga
Attn AMSRL-SE-EP J Nemarich
Attn AMSRL-WT Chf Scntst
Attn AMSRL-WT-NG B McLean
Attn AMSRL-WT-NG Chf

75